

**ThermoML^{*} – an XML-based Approach for Storage and Exchange of Experimental
and Critically Evaluated Thermophysical and
Thermochemical Property Data.**

3. Critically Evaluated Data, Predicted Data, and Equation Representation^{}
(Supporting Information)**

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^{*} "ThermoML" is the reserved namespace for the XML-based IUPAC standard for experimental and critically-evaluated thermodynamic property data storage and capture (<http://www.iupac.org/namespaces/ThermoML/>)

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Supporting Information

Sample ThermoML File #1: *Predicted Data*.

The following ThermoML file contains the predicted critical temperature for 2,3-dihydrobenzo[b]thiophene reported by Steele *et al.*¹ The article includes extensive experimental results, but only the one predicted value is given in the file here.

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xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoML.xsd">
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    <sAuthor2>chi</sAuthor2>
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  <eSourceType>Original</eSourceType>
  <sAuthor>Steele, W. V.[William V.]</sAuthor>
  <sAuthor>Chirico, R. D.[Robert D.]</sAuthor>
  <sAuthor>Cowell, A. B.</sAuthor>
  <sAuthor>Nguyen, A.</sAuthor>
  <sAuthor>Knipmeyer, S. E.</sAuthor>
  <sPubName>J. Chem. Thermodyn.</sPubName>
  <yrPubYr>2003</yrPubYr>
  <dateCit>2004-02-23</dateCit>
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  <sVol>35</sVol>
  <sPage>1253-1276</sPage>
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</RegNum>
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<sContributor>TRC</sContributor>
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<sAuthor>Poling, B. E.[Bruce E.]</sAuthor>
<sAuthor>O'Connell, J.</sAuthor>
<sAuthor>Prausnitz, J. M.[John M.]</sAuthor>
<sPubName>The Properties of Gases and Liquids</sPubName>
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```

Sample ThermoML File #2: *Equation Representation*.

The following ThermoML file contains an example of equation representation. Vapor pressures of 2-methylpyridine were represented by Chirico *et al.*² with the following form of the Wagner equation.

$$\ln(p/p_c) = T_c/T (A_1 \cdot \tau + A_2 \cdot \tau^{1.5} + A_3 \cdot \tau^2 + A_4 \cdot \tau^4)$$

The valid temperature range for the representation, 249.75 K to 639.7 K, is included in the ThermoML file.

```
<?xml version="1.0" encoding="UTF-8"?>
<!-Created by Guided Data Capture (GDC) Software (http://www.trc.nist.gov)-->
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xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoML.xsd">
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  <nVersionMinor>0</nVersionMinor>
</Version>
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    <sAuthor1>chi</sAuthor1>
    <sAuthor2>kni</sAuthor2>
    <nAuthorn>1</nAuthorn>
  </TRCRefID>
  <eType>journal</eType>
  <eSourceType>Original</eSourceType>
  <sAuthor>Chirico, R. D.[Robert D.]</sAuthor>
  <sAuthor>Knipmeyer, S. E.</sAuthor>
  <sAuthor>Nguyen, A.</sAuthor>
  <sAuthor>Steele, W. V.[William V.]</sAuthor>
  <sPubName>J. Chem. Thermodyn.</sPubName>
  <yrPubYr>1999</yrPubYr>
  <dateCit>2004-02-23</dateCit>
  <sTitle>Thermodynamic properties of the methylpyridines. Part 2. Vapor pressures, heat capacities, critical properties, derived thermodynamic functions between the temperatures 250 K and 560 K, and equilibrium isomer distributions for all temperatures >= 250 K</sTitle>
  <sVol>31</sVol>
  <sPage>339-378</sPage>
</Citation>
```

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  </RegNum>
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  <sFormulaMolec>C6H7N</sFormulaMolec>
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```

```

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```

Sample ThermoML File #3: Critically evaluated data together with equation representation including covariance information

The following ThermoML file contains vapor pressure values for pyrrole that were critically evaluated at TRC. The file also contains an equation representation of the vapor pressures with the Wagner equation:

$$\ln(p) - \ln(p_c) = T_c/T (A_1 \cdot \tau + A_2 \cdot \tau^{1.5} + A_3 \cdot \tau^{2.5} + A_4 \cdot \tau^5)$$

The parameters A₁ through A₄ were adjusted in the fit and the elements of the covariance matrix are included in the ThermoML file.

```
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</Citation>
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  </RegNum>
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</Compound>
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          </MultiProp>
        </CriticalEvaluation>
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    </PropertyGroup>
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</DataReport>
```

ThermoML Equation Definitions:

ThermoML.PolynomialExpansion

Name	ThermoML.PolynomialExpansion
Comment	The equation expands Y as a function of one variable X to the number of terms <i>nTerms</i> with coefficients <i>a</i> .
Reference	None
Variable Y	Target property
Variable X	Variable, usually Temperature

$$Y = \sum_{i=0}^{nTerms-1} a_{i+1} \cdot X^i$$

```

<?xml version="1.0" encoding="UTF-8"?>
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xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
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    <nVersionMinor>0</nVersionMinor>
  </Version>
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  <sEqDescription>The equation expands Y as a function of one variable X to the
number of terms nTerms with coefficients A[]</sEqDescription>
  <EqVariable>
    <sEqSymbol>Y</sEqSymbol>
    <sEqVarComment>Target property</sEqVarComment>
  </EqVariable>
  <EqVariable>
    <sEqSymbol>X</sEqSymbol>
    <sEqVarComment>Variable, usually Temperature</sEqVarComment>
  </EqVariable>
  <EqParameter>
    <sEqParSymbol>A</sEqParSymbol>
  </EqParameter>
  <EqConstant>
    <sEqConstantSymbol>nTerms</sEqConstantSymbol>
  </EqConstant>
  <EqMathContent>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <declare type="vector"><ci>A</ci></declare>

```

```

<apply>
  <eq/>
  <ci>Y</ci>
  <apply>
    <sum/>
    <bvar><ci>i</ci></bvar>
    <lowlimit><cn>0</cn></lowlimit>
    <uplimit>
      <apply>
        <minus/>
        <ci>nTerms</ci>
        <cn>1</cn>
      </apply>
    </uplimit>
    <apply>
      <times/>
      <apply>
        <selector/>
        <ci type="vector">A</ci>
        <apply>
          <plus/>
          <ci>i</ci>
          <cn>1</cn>
        </apply>
      </apply>
      <apply>
        <power/>
        <ci>X</ci>
        <ci>i</ci>
      </apply>
    </apply>
  </apply>
</math>
</EqMathContent>
</ThermoMLEquation>

```

ThermoML.CustomExpansion

Name	ThermoML.CustomExpansion
Comment	The equation expands Y as a function of one variable X to the number of terms $nTerms$ with powers n and coefficients a .
Reference	None
Variable Y	Target property
Variable X	Variable, usually Temperature

$$Y = \sum_{i=1}^{nTerms} a_i \cdot X^{ni}$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
<Version>
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  <nVersionMinor>0</nVersionMinor>
</Version>
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<sEqDescription>The equation expands Y as a function of one variable X to the
number of terms nTerms with powers n[] and coefficients A[]</sEqDescription>
<EqVariable>
  <sEqSymbol>Y</sEqSymbol>
  <sEqVarComment>Target property</sEqVarComment>
</EqVariable>
<EqVariable>
  <sEqSymbol>X</sEqSymbol>
  <sEqVarComment>Variable, usually Temperature</sEqVarComment>
</EqVariable>
<EqParameter>
  <sEqParSymbol>A</sEqParSymbol>
</EqParameter>
<EqConstant>
  <sEqConstantSymbol>nTerms</sEqConstantSymbol>
</EqConstant>
<EqConstant>
  <sEqConstantSymbol>n</sEqConstantSymbol>
</EqConstant>
<EqMathContent>
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <declare type="vector"><ci>A</ci></declare>

```

```

<declare type="vector"><ci>n</ci></declare>
<apply>
  <eq/>
  <ci>Y</ci>
  <apply>
    <sum/>
    <bvar><ci>i</ci></bvar>
    <lowlimit><cn>1</cn></lowlimit>
    <uplimit><ci>nTerms</ci></uplimit>
    <apply>
      <times/>
      <apply>
        <selector/>
        <ci type="vector">A</ci>
        <ci>i</ci>
      </apply>
      <apply>
        <power/>
        <ci>X</ci>
        <apply>
          <selector/>
          <ci type="vector">n</ci>
          <ci>i</ci>
        </apply>
        </apply>
      </apply>
    </apply>
  </apply>
</math>
</EqMathContent>
</ThermoMLEquation>

```

ThermoML.Antoine.VaporPressure

Name	ThermoML.Antoine.VaporPressure
Comment	None
Reference	None
Variable p	Vapor pressure
Variable T	Temperature

$$\ln(p/p^\circ) = A + B/(T + C)$$

$$p^\circ = 1 \text{ kPa}$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
<Version>
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</Version>
<sEqName>ThermoML.Antoine.VaporPressure</sEqName>
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  <sEqVarComment>Vapor pressure</sEqVarComment>
</EqVariable>
<EqVariable>
  <sEqSymbol>T</sEqSymbol>
  <sEqVarComment>Temperature</sEqVarComment>
</EqVariable>
<EqParameter>
  <sEqParSymbol>A</sEqParSymbol>
</EqParameter>
<EqParameter>
  <sEqParSymbol>B</sEqParSymbol>
</EqParameter>
<EqParameter>
  <sEqParSymbol>C</sEqParSymbol>
</EqParameter>
<EqMathContent>
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <apply>
      <eq/>
      <apply>

```

```
<ln/>
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</apply>
<apply>
<plus/>
<ci>A</ci>
<apply>
<divide/>
<ci>B</ci>
<apply>
<plus/>
<ci>T</ci>
<ci>C</ci>
</apply>
</apply>
</apply>
</math>
</EqMathContent>
</ThermoMLEquation>
```

ThermoML.WagnerLinear.VaporPressure

Name	ThermoML.WagnerLinear.VaporPressure
Comment	The equation is used for representation of vapor pressure over the liquid. Linear with respect to all adjustable parameters. Allows any number of terms with powers given as constants.
Reference	Wagner, W.[Wolfgang], “New vapour pressure measurements for argon and nitrogen and a new method for establishing rational vapour pressure equations.” <i>Cryogenics</i> 1973 , <i>13</i> , 470-482
Variable p	Vapor pressure
Variable T	Temperature
Variable T_c	Critical temperature
Variable $\ln p_c$	Natural logarithm of critical pressure

$$\tau = 1 - T/T_c$$

$$\ln(p/p^\circ) - \ln(p_c/p^\circ) = T_c/T \cdot \sum_{i=1}^{nTerms} A_i \cdot \tau^{n_i}$$

$$p^\circ = 1 \text{ kPa}$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
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<EqReference>
  <TRCRefID>
    <yrYrPub>1973</yrYrPub>
    <sAuthor1>wag</sAuthor1>
    <sAuthor2></sAuthor2>
    <nAuthorn>0</nAuthorn>
  </TRCRefID>
  <eType>journal</eType>
  <eSourceType>Original</eSourceType>

```

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<sAuthor>Wagner, W.[Wolfgang]</sAuthor>
<sPubName>Cryogenics</sPubName>
<yrPubYr>1973</yrPubYr>
<dateCit>2004-02-20</dateCit>
<sTitle>New vapour pressure measurements for argon and nitrogen and a new method
for establishing rational vapour pressure equations</sTitle>
<sVol>13</sVol>
<sPage>470-82</sPage>
</EqReference>
<EqVariable>
  <sEqSymbol>P</sEqSymbol>
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<EqVariable>
  <sEqSymbol>T</sEqSymbol>
  <sEqVarComment>Temperature</sEqVarComment>
</EqVariable>
<EqParameter>
  <sEqParSymbol>TC</sEqParSymbol>
  <sEqParComment>Critical temperature</sEqParComment>
</EqParameter>
<EqParameter>
  <sEqParSymbol>lnPC</sEqParSymbol>
  <sEqParComment>Natural logarithm of critical pressure</sEqParComment>
</EqParameter>
<EqParameter>
  <sEqParSymbol>A</sEqParSymbol>
</EqParameter>
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  <sEqConstantSymbol>nTerms</sEqConstantSymbol>
</EqConstant>
<EqConstant>
  <sEqConstantSymbol>n</sEqConstantSymbol>
</EqConstant>
<EqMathContent>
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <declare type="vector"><ci>A</ci></declare>
    <declare type="vector"><ci>n</ci></declare>
    <apply>
      <eq/>
      <ci>Tau</ci>
      <apply>
        <minus/>

```

```

<cn>1</cn>
<apply>
  <divide/>
  <ci>T</ci>
  <ci>TC</ci>
</apply>
</apply>
<apply>
  <eq/>
  <apply>
    <minus/>
    <apply>
      <ln/>
      <ci>P</ci>
    </apply>
    <ci>lnPC</ci>
  </apply>
<apply>
  <divide/>
  <apply>
    <sum/>
    <bvar><ci>i</ci></bvar>
    <lowlimit><cn>1</cn></lowlimit>
    <uplimit><ci>nTerms</ci></uplimit>
    <apply>
      <times/>
      <apply>
        <selector/>
        <ci type="vector">A</ci>
        <ci>i</ci>
      </apply>
      <apply>
        <power/>
        <ci>Tau</ci>
      <apply>
        <selector/>
        <ci type="vector">n</ci>
        <ci>i</ci>
      </apply>
    </apply>
  </apply>
</apply>
</apply>

```

```
<apply>
  <divide/>
  <ci>T</ci>
  <ci>TC</ci>
</apply>
</apply>
</math>
</EqMathContent>
</ThermoMLEquation>
```

ThermoML.Wagner25Linear.VaporPressure

Name	ThermoML.Wagner25Linear.VaporPressure
Comment	The equation is used for representation of vapor pressure over the liquid. Linear with respect to all adjustable parameters.
Reference	Ambrose, D.; Ewing, M. B.; Ghassee N. B.; Sanchez Ochoa, J. C., "The ebulliometric method of vapor-pressure measurement: vapor pressures of benzene, hexafluorobenzene, and naphthalene." <i>J. Chem. Thermodyn.</i> 1990 , 22, 589.
Variable p	Vapor pressure
Variable T	Temperature
Variable T_c	Critical temperature
Variable $\ln(p_c)$	Natural logarithm of critical pressure

$$\tau = 1 - T/T_c$$

$$\ln(p/p^\circ) - \ln(p_c/p^\circ) = T_c/T (A_1 \cdot \tau + A_2 \cdot \tau^{1.5} + A_3 \cdot \tau^{2.5} + A_4 \cdot \tau^5)$$

$$p^\circ = 1 \text{ kPa}$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
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liquid. Linear with respect to all adjustable parameters.</sEqDescription>
  <EqReference>
    <TRCRefID>
      <yrYrPub>1990</yrYrPub>
      <sAuthor1>amb</sAuthor1>
      <sAuthor2>ewi</sAuthor2>
      <nAuthorn>0</nAuthorn>
    </TRCRefID>
    <eType>journal</eType>
    <eSourceType>Original</eSourceType>
    <sAuthor>Ambrose, D.</sAuthor>
    <sAuthor>Ewing, M. B.</sAuthor>
  
```

```

<sAuthor>Ghiassee N. B.</sAuthor>
<sAuthor>Sanchez Ochoa, J. C.</sAuthor>
<sPubName>J. Chem. Thermodyn.</sPubName>
<yrPubYr>1990</yrPubYr>
<sTitle>The ebulliometric method of vapor-pressure measurement: vapor pressures of
benzene, hexafluorobenzene, and naphthalene</sTitle>
<sVol>22</sVol>
<sPage>589</sPage>
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  <sEqVarComment>Temperature</sEqVarComment>
</EqVariable>
<EqParameter>
  <sEqParSymbol>TC</sEqParSymbol>
  <sEqParComment>Critical temperature</sEqParComment>
</EqParameter>
<EqParameter>
  <sEqParSymbol>lnPC</sEqParSymbol>
  <sEqParComment>Natural logarithm of critical pressure</sEqParComment>
</EqParameter>
<EqParameter>
  <sEqParSymbol>A</sEqParSymbol>
</EqParameter>
<EqMathContent>
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  <declare type="vector" nargs="4"><ci>A</ci></declare>
  <declare>
    <ci>n</ci>
    <vector>
      <cn>1</cn>
      <cn>1.5</cn>
      <cn>2.5</cn>
      <cn>5</cn>
    </vector>
  </declare>
  <apply>
    <eq/>
    <ci>Tau</ci>

```

```

<apply>
  <minus/>
  <cn>1</cn>
  <apply>
    <divide/>
    <ci>T</ci>
    <ci>TC</ci>
  </apply>
</apply>
<apply>
  <eq/>
  <apply>
    <minus/>
    <apply>
      <ln/>
      <ci>P</ci>
    </apply>
    <ci>lnPC</ci>
  </apply>
  <apply>
    <divide/>
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      <uplimit><cn>4</cn></uplimit>
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      <times/>
      <apply>
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        <ci type="vector">A</ci>
        <ci>i</ci>
      </apply>
      <apply>
        <power/>
        <ci>Tau</ci>
      <apply>
        <selector/>
        <ci type="vector">n</ci>
        <ci>i</ci>
      </apply>
    </apply>
  </apply>
</apply>

```

```
</apply>
</apply>
<apply>
  <divide/>
  <ci>T</ci>
  <ci>TC</ci>
</apply>
</apply>
</math>
</EqMathContent>
</ThermoMLEquation>
```

ThermoML.Wagner36Linear.VaporPressure

Name	ThermoML.Wagner36Linear.VaporPressure
Comment	The equation is used for representation of vapor pressure over the liquid. Linear with respect to all adjustable parameters. Allows any number of terms with powers given as constants.
Reference	Wagner, W.[Wolfgang], “New vapour pressure measurements for argon and nitrogen and a new method for establishing rational vapour pressure equations.” <i>Cryogenics</i> 1973 , 13, 470-482.
Variable p	Vapor pressure
Variable T	Temperature
Variable T_c	Critical temperature
Variable $\ln(p_c)$	Natural logarithm of critical pressure

$$\tau = 1 - T/T_c$$

$$\ln(p/p^\circ) - \ln(p_c/p^\circ) = T_c/T (A_1 \cdot \tau + A_2 \cdot \tau^{1.5} + A_3 \cdot \tau^3 + A_4 \cdot \tau^6)$$

$$p^\circ = 1 \text{ kPa}$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
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</Version>
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liquid. Linear with respect to all adjustable parameters.</sEqDescription>
<EqReference>
  <TRCRefID>
    <yrYrPub>1973</yrYrPub>
    <sAuthor1>wag</sAuthor1>
    <sAuthor2></sAuthor2>
    <nAuthorn>0</nAuthorn>
  </TRCRefID>
  <eType>journal</eType>
  <eSourceType>Original</eSourceType>
  <sAuthor>Wagner, W.[Wolfgang]</sAuthor>

```

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<sPubName>Cryogenics</sPubName>
<yrPubYr>1973</yrPubYr>
<dateCit>2004-02-20</dateCit>
<sTitle>New vapour pressure measurements for argon and nitrogen and a new method
for establishing rational vapour pressure equations</sTitle>
<sVol>13</sVol>
<sPage>470-82</sPage>
</EqReference>
<EqVariable>
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<sEqVarComment>Vapor pressure</sEqVarComment>
</EqVariable>
<EqVariable>
<sEqSymbol>T</sEqSymbol>
<sEqVarComment>Temperature</sEqVarComment>
</EqVariable>
<EqParameter>
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<sEqParComment>Critical temperature</sEqParComment>
</EqParameter>
<EqParameter>
<sEqParSymbol>lnPC</sEqParSymbol>
<sEqParComment>Natural logarithm of critical pressure</sEqParComment>
</EqParameter>
<EqParameter>
<sEqParSymbol>A</sEqParSymbol>
</EqParameter>
<EqMathContent>
<math xmlns="http://www.w3.org/1998/Math/MathML">
<declare type="vector" nargs="4"><ci>A</ci></declare>
<declare>
<ci>n</ci>
<vector>
<cn>1</cn>
<cn>1.5</cn>
<cn>3</cn>
<cn>6</cn>
</vector>
</declare>
<apply>
<eq/>
<ci>Tau</ci>
<apply>

```

```

<minus/>
<cn>1</cn>
<apply>
  <divide/>
  <ci>T</ci>
  <ci>TC</ci>
</apply>
</apply>
</apply>
<eq/>
<apply>
  <minus/>
  <apply>
    <ln/>
    <ci>P</ci>
  </apply>
  <ci>lnPC</ci>
</apply>
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  <divide/>
  <apply>
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    <uplimit><cn>4</cn></uplimit>
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  <times/>
  <apply>
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    <ci type="vector">A</ci>
    <ci>i</ci>
  </apply>
  <apply>
    <power/>
    <ci>Tau</ci>
  <apply>
    <selector/>
    <ci type="vector">n</ci>
    <ci>i</ci>
  </apply>
</apply>
</apply>

```

```
</apply>
<apply>
  <divide/>
  <ci>T</ci>
  <ci>TC</ci>
</apply>
</apply>
</apply>
</math>
</EqMathContent>
</ThermoMLEquation>
```

ThermoML.Helmholtz3General.EOS

Name	ThermoML.Helmholtz3General.EOS
Comment	The equation represents the non-ideal part of the Helmholtz energy as a function of temperature and density.
Reference	Lemmon, E.[Eric] W.; Jacobsen, R.[Richard] T. “An International Standard Formulation for the Thermodynamic Properties of 1,1,1-Trifluoroethane (HFC-143a) for Temperatures from 161 to 450 K and Pressures to 50 MPa.” <i>J. Phys. Chem. Ref. Data</i> 2000 , 29, 521-552.
Variable A^r	Helmholtz energy (in $\text{kJ}\cdot\text{mol}^{-1}$) expressed as the difference between the real fluid and the ideal-gas at the same temperature and density.
Variable T	Temperature
Variable ρ	Density
Variable T_c	Critical temperature
Variable ρ_c	Critical density
Constant R	Gas constant expressed in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
Constant e	This constant does not appear in the original formulation. It is added here for uniform representation of all equation terms. Its value is 0 or -1, depending on the necessity of the exponential density factor in the term

$$\tau = T_c/T \text{ and } \delta = \rho/\rho_c$$

$$1000 \cdot A^r / (RT) = \sum_{i=1}^{nTerms} n_i \cdot \delta^{di} \cdot \tau^{ti} \cdot \exp(e_i \cdot \delta^{pi})$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
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  <nVersionMinor>0</nVersionMinor>
</Version>
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<sEqDescription>The equation represents the non-ideal part of the Helmholtz energy as a function of temperature and density.</sEqDescription>
<EqReference>
  <eType>journal</eType>
  <sAuthor>Lemmon, E.[Eric]</sAuthor>
  <sAuthor>Jacobsen, R.[Richard]</sAuthor>
  <sPubName>J. Phys. Chem. Ref. Data</sPubName>
  <yrPubYr>2000</yrPubYr>

```

<sTitle>An International Standard Formulation for the Thermodynamic Properties of
 1,1,1-Trifluoroethane (HFC-143a) for Temperatures from 161 to 450 K and Pressures to
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 <sVol>29</sVol>
 <sPage>521-552</sPage>
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 <EqParameter>
 <sEqParSymbol>DC</sEqParSymbol>
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 <EqParameter>
 <sEqParSymbol>n</sEqParSymbol>
 </EqParameter>
 <EqConstant>
 <sEqConstantSymbol>R</sEqConstantSymbol>
 <sEqConstantComment>Gas constant expressed in
 J/(K*mol)</sEqConstantComment>
 </EqConstant>
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 <sEqConstantSymbol>nTerms</sEqConstantSymbol>
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 </EqConstant>
 <EqConstant>
 <sEqConstantSymbol>t</sEqConstantSymbol>

```

</EqConstant>
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is added here for uniform representation of all equation terms. Its value is 0 or -1,
depending on the necessity of the exponential density factor in the
term</sEqConstantComment>
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</EqConstant>
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  </declare>
  <declare type="vector">
    <ci>t</ci>
  </declare>
  <declare type="vector">
    <ci>e</ci>
  </declare>
  <declare type="vector">
    <ci>p</ci>
  </declare>
  <apply>
    <eq/>
    <ci>Tau</ci>
    <apply>
      <divide/>
      <ci>TC</ci>
      <ci>T</ci>
    </apply>
  </apply>
  <apply>
    <eq/>
    <ci>Delta</ci>
    <apply>
      <divide/>
      <ci>Density</ci>
      <ci>DC</ci>
    </apply>
  </apply>
</math>

```

```

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  <apply>
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    <apply>
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      <apply>
        <times/>
        <cn>R</cn>
        <ci>T</ci>
      </apply>
    </apply>
  </apply>
  <apply>
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    <bvar><ci>i</ci></bvar>
    <lowlimit><cn>1</cn></lowlimit>
    <uplimit><ci>nTerms</ci></uplimit>
    <apply>
      <times/>
      <apply>
        <selector/>
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        <ci>i</ci>
      </apply>
    <apply>
      <times/>
      <apply>
        <power/>
        <ci>Delta</ci>
        <apply>
          <selector/>
          <ci type="vector">d</ci>
          <ci>i</ci>
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      </apply>
    <apply>
      <times/>
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    </apply>
  </apply>

```

```

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      <apply>
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</ThermoMLEquation>

```

ThermoML.Helmholtz4General.EOS

Name	ThermoML.Helmholtz4General.EOS
Comment	The equation represents the non-ideal part of the Helmholtz energy as a function of temperature and density.
Reference	Lemmon, E.[Eric] W.; Jacobsen, R.[Richard] T. “A New Functional Form and New Fitting Techniques for Equations of State with Application to Pentafluoroethane (HFC-125),” <i>J. Phys. Chem. Ref. Data.</i> 2004 . In press.
Variable A'	Helmholtz energy (in $\text{kJ}\cdot\text{mol}^{-1}$) expressed as the difference between the real fluid and the ideal-gas at the same temperature and density
Variable T	Temperature
Variable ρ	Density
Variable T_c	Critical temperature
Variable ρ_c	Critical density
Constant R	Gas constant expressed in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
Constant e_d	This constant does not appear in the original formulation. It is added here for uniform representation of all equation terms. Its value is 0 or -1, depending on the necessity of the exponential density factor in the term
Constant e_t	This constant does not appear in the original formulation. It is added here for uniform representation of all equation terms. Its value is 0 or -1, depending on the necessity of the exponential temperature factor in the term

$$\tau = T_c/T \text{ and } \delta = \rho/\rho_c$$

$$1000 \cdot A' / (RT) = \sum_{i=1}^{nTerms} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp(e_{d_i} \cdot \delta^{p_i}) \cdot \exp(e_{t_i} \cdot \tau^{q_i})$$

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    <nVersionMajor>1</nVersionMajor>
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  <sEqDescription>The equation represents the non-ideal part of the Helmholtz energy as
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  <EqReference>
    <eType>journal</eType>
    <sAuthor>Lemmon, E.[Eric]</sAuthor>
  
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<sAuthor>Jacobsen, R.[Richard]</sAuthor>
 <sPubName>J. Phys. Chem. Ref. Data</sPubName>
 <yrPubYr>2004</yrPubYr>
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 <sVol>33</sVol>
 <sPage>In press</sPage>
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    <apply>
      <times/>

```

```

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```

```

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```

ThermoML.SpanWagner12Nonpolar.EOS

Name	ThermoML.SpanWagner12Nonpolar.EOS
Comment	The equation represents the non-ideal part of the Helmholtz energy as a function of temperature and density.
Reference	Span, R.[Roland]; Wagner, W.[Wolfgang] “Equations of State for Technical Applications. II. Results for Nonpolar Fluids,” <i>Int. J. Thermophys.</i> 2003 , 24, 41-109.
Variable A'	Helmholtz energy (in $\text{kJ}\cdot\text{mol}^{-1}$) expressed as the difference between the real fluid and the ideal-gas at the same temperature and density
Variable T	Temperature
Variable ρ	Density
Variable T_c	Critical temperature
Variable ρ_c	Critical density
Constant R	Gas constant expressed in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
Constant e	This constant does not appear in the original formulation. It is added here for uniform representation of all equation terms. Its value is 0 or -1, depending on the necessity of the exponential density factor in the term

$$\tau = T_c/T; \delta = \rho/\rho_c$$

$$1000 \cdot A' / (RT) = \sum_{i=1}^{12} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp(e_i \cdot \delta^{p_i})$$

Equation constant arrays:

$$d = (1, 1, 1, 2, 3, 7, 2, 5, 1, 4, 3, 4)$$

$$t = (0.250, 1.125, 1.500, 1.375, 0.250, 0.875, 0.625, 1.750, 3.625, 3.625, 14.5, 12.0)$$

$$e = (0, 0, 0, 0, 0, -1, -1, -1, -1, -1)$$

$$p = (0, 0, 0, 0, 0, 1, 1, 2, 2, 3, 3)$$

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  <EqReference>
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<eType>journal</eType>
<sAuthor>Span, R.[Roland]</sAuthor>
<sAuthor>Wagner, W.[Wolfgang]</sAuthor>
<sPubName>Int. J. Thermophys.</sPubName>
<yrPubYr>2003</yrPubYr>
<sTitle>Equations of State for Technical Applications. II. Results for Nonpolar
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<sVol>24</sVol>
<sPage>41-109</sPage>
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```

```

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    <times/>
    <apply>
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ThermoML.SpanWagner12Polar.EOS

Name	ThermoML.SpanWagner12Polar.EOS
Comment	The equation represents the non-ideal part of the Helmholtz energy as a function of temperature and density.
Reference	Span, R.[Roland]; Wagner, W.[Wolfgang], "Equations of State for Technical Applications. III. Results for Polar Fluids," <i>Int. J. Thermophys.</i> 2003 , 24, 111-161.
Variable A^r	Helmholtz energy (in $\text{kJ}\cdot\text{mol}^{-1}$) expressed as the difference between the real fluid and the ideal-gas at the same temperature and density
Variable T	Temperature
Variable ρ	Density
Variable T_c	Critical temperature
Variable ρ_c	Critical density
Constant R	Gas constant expressed in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
Constant e	This constant does not appear in the original formulation. It is added here for uniform representation of all equation terms. Its value is 0 or -1, depending on the necessity of the exponential density factor in the term

$$\tau = T_c/T; \delta = \rho/\rho_c$$

$$1000 \cdot A^r / (RT) = \sum_{i=1}^{12} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp(e_i \cdot \delta^{p_i})$$

Equation constant arrays:

$$d = (1, 1, 1, 3, 7, 1, 2, 5, 1, 1, 4, 2)$$

$$t = (0.250, 1.250, 1.500, 0.250, 0.875, 2.375, 2.000, 2.125, 3.500, 6.50, 4.75, 12.5)$$

$$e = (0, 0, 0, 0, -1, -1, -1, -1, -1, -1)$$

$$p = (0, 0, 0, 0, 1, 1, 1, 2, 2, 2, 3)$$

```

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 <sAuthor>Wagner, W.[Wolfgang]</sAuthor>
 <sPubName>Int. J. Thermophys.</sPubName>
 <yrPubYr>2003</yrPubYr>
 <sTitle>Equations of State for Technical Applications. III. Results for Polar Fluids</sTitle>
 <sVol>24</sVol>
 <sPage>111-161</sPage>

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```

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</EqMathContent>
</ThermoMLEquation>

```

ThermoML.HelmholtzIG.EOS

Name	ThermoML.HelmholtzIG.EOS
Comment	The equation represents the ideal-gas Helmholtz energy as a function of temperature and density. Only differences between two states should be calculated with this equation.
Reference	Span, R.[Roland]; Wagner, W.[Wolfgang], “A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple Point Temperature to 1100 K at Pressures up to 800 MPa.” <i>J. Phys. Chem. Ref. Data</i> 1996 , 25, 1509-1596.
Reference	Span, R.[Roland]; Lemmon, E.[Eric]; Jacobsen, R.[Richard]; Wagner, W.[Wolfgang]; Yokozeki, A.[Akimichi] “A Reference Equation of State for the Thermodynamic Properties of Nitrogen for Temperatures from 63.151 to 1000 K at Pressures up to 2200 MPa.” <i>J. Phys. Chem. Ref. Data</i> 2000 , 29, 1361-1433.
Reference	Lemmon, E.[Eric] W.; Jacobsen, R.[Richard] T. “An International Standard Formulation for the Thermodynamic Properties of 1,1,1-Trifluoroethane (HFC-143a) for Temperatures from 161 to 450 K and Pressures to 50 MPa.” <i>J. Phys. Chem. Ref. Data</i> 2000 , 29, 521-552.
Variable A°	Helmholtz energy (in $\text{kJ}\cdot\text{mol}^{-1}$) of the ideal gas
Variable T	Temperature
Variable ρ	Density
Variable T_c	Critical temperature
Variable ρ_c	Critical density
Constant R	Gas constant expressed in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$$\tau = T_c/T; \delta = \rho/\rho_c$$

$$1000 \cdot A^\circ / (RT) = \ln(\delta) + t \cdot \ln(\tau) + \sum_{i=1}^{nA} a_i \cdot \tau^{n_i} + \sum_{i=1}^{nB} b_i \cdot \ln[1 - \exp(-c_i \cdot \tau)]$$

```

<?xml version="1.0" encoding="UTF-8"?>
<ThermoMLEquation xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:noNamespaceSchemaLocation="http://trc.nist.gov/ThermoMLEquation.xsd">
  <Version>
    <nVersionMajor>1</nVersionMajor>
    <nVersionMinor>0</nVersionMinor>
  </Version>
  <sEqName>ThermoML.HelmholtzIG.EOS</sEqName>
  <sEqDescription>The equation represents the ideal-gas Helmholtz energy as a function
of temperature and density. Only differences between two states should be calculated
with this equation.</sEqDescription>

```

```

<EqReference>
  <eType>journal</eType>
  <sAuthor>Span, R.[Roland]</sAuthor>
  <sAuthor>Wagner, W.[Wolfgang]</sAuthor>
  <sPubName>J. Phys. Chem. Ref. Data</sPubName>
  <yrPubYr>1996</yrPubYr>
  <sTitle>A New Equation of State for Carbon Dioxide Covering the Fluid Region from
the Triple Point Temperature to 1100 K at Pressures up to 800 MPa</sTitle>
  <sVol>25</sVol>
  <sPage>1509-1596</sPage>
</EqReference>
<EqReference>
  <eType>journal</eType>
  <sAuthor>Span, R.[Roland]</sAuthor>
  <sAuthor>Lemmon, E.[Eric]</sAuthor>
  <sAuthor>Jacobsen, R.[Richard]</sAuthor>
  <sAuthor>Wagner, W.[Wolfgang]</sAuthor>
  <sAuthor>Yokozeki, A.[Akimichi]</sAuthor>
  <sPubName>J. Phys. Chem. Ref. Data</sPubName>
  <yrPubYr>2000</yrPubYr>
  <sTitle>A Reference Equation of State for the Thermodynamic Properties of Nitrogen
for Temperatures from 63.151 to 1000 K at Pressures up to 2200 MPa</sTitle>
  <sVol>29</sVol>
  <sPage>1361-1433</sPage>
</EqReference>
<EqReference>
  <eType>journal</eType>
  <sAuthor>Lemmon, E.[Eric]</sAuthor>
  <sAuthor>Jacobsen, R.[Richard]</sAuthor>
  <sPubName>J. Phys. Chem. Ref. Data</sPubName>
  <yrPubYr>2000</yrPubYr>
  <sTitle>An International Standard Formulation for the Thermodynamic Properties of
1,1,1-Trifluoroethane (HFC-143a) for Temperatures from 161 to 450 K and Pressures to
50 MPa</sTitle>
  <sVol>29</sVol>
  <sPage>521-552</sPage>
</EqReference>
<EqVariable>
  <sEqSymbol>A0</sEqSymbol>
  <sEqVarComment>Helmholtz energy</sEqVarComment>
</EqVariable>
<EqVariable>
  <sEqSymbol>T</sEqSymbol>

```

```

<sEqVarComment>Temperature</sEqVarComment>
</EqVariable>
<EqVariable>
  <sEqSymbol>Density</sEqSymbol>
  <sEqVarComment>Density</sEqvarComment>
</EqVariable>
<EqParameter>
  <sEqParSymbol>TC</sEqParSymbol>
  <sEqParComment>Critical temparature</sEqParComment>
</EqParameter>
<EqParameter>
  <sEqParSymbol>DC</sEqParSymbol>
  <sEqParComment>Critical density</sEqParComment>
</EqParameter>
<EqParameter>
  <sEqParSymbol>t</sEqParSymbol>
</EqParameter>
<EqParameter>
  <sEqParSymbol>a</sEqParSymbol>
</EqParameter>
<EqParameter>
  <sEqParSymbol>b</sEqParSymbol>
</EqParameter>
<EqParameter>
  <sEqParSymbol>c</sEqParSymbol>
</EqParameter>
<EqConstant>
  <sEqConstantSymbol>R</sEqConstantSymbol>
  <sEqConstantComment>Gas constant expressed in
J/(K*mol)</sEqConstantComment>
</EqConstant>
<EqConstant>
  <sEqConstantSymbol>nA</sEqConstantSymbol>
</EqConstant>
<EqConstant>
  <sEqConstantSymbol>nB</sEqConstantSymbol>
</EqConstant>
<EqMathContent>
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <declare type="vector">
      <ci>a</ci>
    </declare>
    <declare type="vector">

```

```

<ci>b</ci>
</declare>
<declare type="vector">
  <ci>c</ci>
</declare>
<apply>
  <eq/>
  <ci>Tau</ci>
  <apply>
    <divide/>
    <ci>TC</ci>
    <ci>T</ci>
  </apply>
</apply>
<apply>
  <eq/>
  <ci>Delta</ci>
  <apply>
    <divide/>
    <ci>Density</ci>
    <ci>DC</ci>
  </apply>
</apply>
<apply>
  <eq/>
  <apply>
    <times/>
    <cn>1000</cn>
    <apply>
      <divide/>
      <ci>A0</ci>
      <apply>
        <times/>
        <cn>R</cn>
        <ci>T</ci>
      </apply>
    </apply>
  </apply>
</apply>
<apply>
  <plus/>
  <apply>
    <ln/>
    <ci>Delta</ci>

```

```

</apply>
<apply>
  <plus/>
  <apply>
    <times/>
    <ci>t</ci>
    <apply>
      <ln/>
      <ci>Tau</ci>
    </apply>
  </apply>
  <apply>
    <plus/>
    <apply>
      <sum/>
      <bvar><ci>i</ci></bvar>
      <lowlimit><cn>1</cn></lowlimit>
      <uplimit><ci>nA</ci></uplimit>
      <apply>
        <times/>
        <apply>
          <selector/>
          <ci type="vector">a</ci>
          <ci>i</ci>
        </apply>
        <apply>
          <power/>
          <ci>Tau</ci>
        <apply>
          <selector/>
          <ci type="vector">n</ci>
          <ci>i</ci>
        </apply>
      </apply>
    </apply>
  </apply>
<apply>
  <sum/>
  <bvar><ci>i</ci></bvar>
  <lowlimit><cn>1</cn></lowlimit>
  <uplimit><ci>nB</ci></uplimit>
  <apply>
    <times/>

```


The complete text of *ThermoMLEquation*

```
<?xml version="1.0" encoding="UTF-8"?>
<xsd:schema
    xmlns:xsd =“http://www.w3.org/2001/XMLSchema”
    xmlns:mml =“http://www.w3.org/1998/Math/MathML”>
    <xsd:annotation>
        <xsd:documentation>Definition of an equation for use with ThermoML. Version 1.0</xsd:documentation>
    </xsd:annotation>
    <xsd:import
        schemaLocation=“http://www.w3.org/Math/XMLSchema/mathml2/mathml2.xsd”
        namespace=“http://www.w3.org/1998/Math/MathML”/>
    <xsd:include schemaLocation="http://trc.nist.gov/ThermoML.xsd"/>
    <xsd:element name="ThermoMLEquation" type="ThermoMLEquation"/>
    <xsd:complexType name="ThermoMLEquation">
        <xsd:annotation>
            <xsd:documentation>Definition and MathML description of an empirical equation</xsd:documentation>
        </xsd:annotation>
        <xsd:sequence>
            <xsd:element name="Version">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element name="nVersionMajor" type="xsd:integer"/>
                        <xsd:element name="nVersionMinor" type="xsd:integer"/>
                    </xsd:sequence>
                </xsd:complexType>
            </xsd:element>
            <xsd:element name="sEqName" type="xsd:string"/>
            <xsd:element name="sEqAltName" type="xsd:string" minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element name="sEqDescription" type="xsd:string" minOccurs="0"/>
            <xsd:element name="EqReference" type="CitationType" minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element name="EqVariable" minOccurs="0" maxOccurs="unbounded">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element name="sEqSymbol" type="xsd:string"/>
                        <xsd:element name="sEqVarComment" type="xsd:string" minOccurs="0"/>
                        <xsd:element name="IUPACSymbol" minOccurs="0">
                            <xsd:complexType>
                                <xsd:sequence>
```

```

        <xsd:element ref="mml:math"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="EqParameter" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="sEqParSymbol" type="xsd:string"/>
            <xsd:element name="sEqParComment" type="xsd:string" minOccurs="0"/>
            <xsd:element name="IUPACSymbol" minOccurs="0">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element ref="mml:math"/>
                    </xsd:sequence>
                </xsd:complexType>
            </xsd:element>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="EqConstant" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="sEqConstantSymbol" type="xsd:string"/>
            <xsd:element name="sEqConstantComment" type="xsd:string"
minOccurs="0"/>
            <xsd:element name="IUPACSymbol" minOccurs="0">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element ref="mml:math"/>
                    </xsd:sequence>
                </xsd:complexType>
            </xsd:element>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="EqMathContent" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element ref="mml:math"/>
        </xsd:sequence>

```

```
</xsd:complexType>
</xsd:element>
<xsd:element name="EqMathPresentation" minOccurs="0"
maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element ref="mml:math"/>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:schema>
```

The complete text of *ThermoML*

```
<?xml version="1.0" encoding="UTF-8"?>
<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema"
elementFormDefault="qualified" attributeFormDefault="unqualified">
  <xsd:annotation>
    <xsd:documentation>ThermoML version 3.0</xsd:documentation>
  </xsd:annotation>
  <xsd:element name="DataReport" type="DataReport"/>
  <xsd:complexType name="DataReport">
    <xsd:annotation>
      <xsd:documentation>TRCReport complex type</xsd:documentation>
    </xsd:annotation>
    <xsd:sequence>
      <xsd:element name="Version">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="nVersionMajor" type="xsd:integer"/>
            <xsd:element name="nVersionMinor" type="xsd:integer"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="Citation" type="CitationType"/>
      <xsd:element ref="Compound" minOccurs="0" maxOccurs="unbounded"/>
      <xsd:element ref="PureOrMixtureData" minOccurs="0" maxOccurs="unbounded"/>
      <xsd:element ref="ReactionData" minOccurs="0" maxOccurs="unbounded"/>
    </xsd:sequence>
  </xsd:complexType>
<!--
-->
<xsd:simpleType name="ECitationType">
  <xsd:annotation>
    <xsd:documentation>Type of citation</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="book"/>
    <xsd:enumeration value="journal"/>
    <xsd:enumeration value="report"/>
    <xsd:enumeration value="patent"/>
    <xsd:enumeration value="thesis"/>
    <xsd:enumeration value="conferenceProceedings"/>
    <xsd:enumeration value="archivedDocument"/>
```

```

<xsd:enumeration value="personalCorrespondence"/>
<xsd:enumeration value="publishedTranslation"/>
<xsd:enumeration value="unspecified"/>
</xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="ECitationSourceType">
<xsd:annotation>
  <xsd:documentation>The status type of the citation</xsd:documentation>
</xsd:annotation>
<xsd:restriction base="xsd:string">
  <xsd:enumeration value="Original"/>
  <xsd:enumeration value="BiblioBulChemThermo"/>
  <xsd:enumeration value="TRCGeneral"/>
  <xsd:enumeration value="TRCGeneralChecked"/>
  <xsd:enumeration value="TRCDataCard"/>
  <xsd:enumeration value="ChemicalAbstracts"/>
  <xsd:enumeration value="Other"/>
</xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="ECitationDataType">
<xsd:annotation>
  <xsd:documentation>The data type of the citation</xsd:documentation>
</xsd:annotation>
<xsd:restriction base="xsd:string">
  <xsd:enumeration value="ReferenceOnly"/>
  <xsd:enumeration value="SomeNumerical"/>
  <xsd:enumeration value="PureOnly"/>
  <xsd:enumeration value="Pure+SomeMixture"/>
  <xsd:enumeration value="MixtureOnly"/>
  <xsd:enumeration value="All"/>
  <xsd:enumeration value="GraphicalOnly"/>
</xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:element name="TRCRefID">

```

```

<xsd:annotation>
  <xsd:documentation>TRC Reference Identifier</xsd:documentation>
</xsd:annotation>
<xsd:complexType>
  <xsd:sequence>
    <xsd:element name="yrYrPub" type="xsd:integer">
      <xsd:annotation>
        <xsd:documentation>Integer year of publication</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sAuthor1" type="xsd:string">
      <xsd:annotation>
        <xsd:documentation>First 3 characters of Author 1 last
name</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sAuthor2" type="xsd:string">
      <xsd:annotation>
        <xsd:documentation>First 3 characters of Author 2 last
name</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="nAuthorn" type="xsd:integer">
      <xsd:annotation>
        <xsd:documentation>Integer identifier to distinguish
conflicts</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
  </xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:complexType name="CitationType">
  <xsd:sequence>
    <xsd:element ref="TRCRefID" minOccurs="0"/>
    <xsd:element name="eType" type="ECitationType" minOccurs="0">
      <xsd:annotation>
        <xsd:documentation>The type of citation</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="eSourceType" type="ECitationSourceType" minOccurs="0">

```

```

<xsd:annotation>
  <xsd:documentation>The source status type for a citation</xsd:documentation>
</xsd:annotation>
</xsd:element>
<xsd:element name="eDataType" type="ECitationDataType" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>The data type of the citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sCompany" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Company, institution, or conference
name</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sAuthor" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">
  <xsd:annotation>
    <xsd:documentation>Author of citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sPubName" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Name of the publication where the citation was
published.</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="yrPubYr" type="xsd:gYear" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Publication year of the citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="dateCit" type="xsd:date" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Date of the citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sTitle" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Title of the citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sAbstract" type="xsd:string" minOccurs="0">

```

```

<xsd:annotation>
  <xsd:documentation>An abstract of the citation</xsd:documentation>
</xsd:annotation>
</xsd:element>
<xsd:element name="sKeyword" type="xsd:string" minOccurs="0"
maxOccurs="unbounded"/>
<xsd:element name="urlCit" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>URL to the citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sCASCit" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>The Chemical Abstracts Service
citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sBulChemThermoCit" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>The Bulletin of Chemical Thermodynamics
citation</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sIDNum" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Identification number, e.g., a patent number or a document
number</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sLocation" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Reference to a location</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sVol" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Volume number</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sPage" type="xsd:string" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Page range where the citation can be
found</xsd:documentation>
  </xsd:annotation>

```

```

    </xsd:annotation>
</xsd:element>
<xsd:choice minOccurs="0">
    <xsd:element name="book">
        <xsd:complexType>
            <xsd:sequence>
                <xsd:element name="sChapter" type="xsd:string" minOccurs="0">
                    <xsd:annotation>
                        <xsd:documentation>Chapter number</xsd:documentation>
                    </xsd:annotation>
                </xsd:element>
                <xsd:element name="sEdition" type="xsd:string" minOccurs="0">
                    <xsd:annotation>
                        <xsd:documentation>Edition number of the book</xsd:documentation>
                    </xsd:annotation>
                </xsd:element>
                <xsd:element name="sEditor" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">
                    <xsd:annotation>
                        <xsd:documentation>Editor of the book</xsd:documentation>
                    </xsd:annotation>
                </xsd:element>
                <xsd:element name="sISBN" type="xsd:string" minOccurs="0">
                    <xsd:annotation>
                        <xsd:documentation>The International Standard Book
Number</xsd:documentation>
                    </xsd:annotation>
                </xsd:element>
                <xsd:element name="sPublisher" type="xsd:string" minOccurs="0">
                    <xsd:annotation>
                        <xsd:documentation>Publisher name and city</xsd:documentation>
                    </xsd:annotation>
                </xsd:element>
            </xsd:sequence>
        </xsd:complexType>
    </xsd:element>
    <xsd:element name="journal">
        <xsd:complexType>
            <xsd:sequence>
                <xsd:element name="sISSN" type="xsd:string" minOccurs="0">
                    <xsd:annotation>
                        <xsd:documentation>The International Standard Subscription
Number</xsd:documentation>

```

```

        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sIssue" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>Issue number, usually indicates
month</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="sCODEN" type="xsd:string" minOccurs="0">
        <xsd:annotation>
            <xsd:documentation>The CODEN identification of the
journal</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="thesis">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="sDeg" type="xsd:string" minOccurs="0">
                <xsd:annotation>
                    <xsd:documentation>Academic degree designation, e.g., MS or
PhD</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="sDegInst" type="xsd:string" minOccurs="0">
                <xsd:annotation>
                    <xsd:documentation>Academic degree granting
institution</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            <xsd:element name="sUMIPubNum" type="xsd:string" minOccurs="0">
                <xsd:annotation>
                    <xsd:documentation>University Microfilms International Publication
Number</xsd:documentation>
                </xsd:annotation>
            </xsd:element>
            </xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:choice>
</xsd:sequence>

```

```

</xsd:complexType>
<!--
-->
<xsd:element name="Compound">
  <xsd:annotation>
    <xsd:documentation>Material component characteristics that serves to identify the
component      </xsd:documentation>
  </xsd:annotation>
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="RegNum">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="nCASRNum" type="xsd:integer" minOccurs="0"/>
            <xsd:element name="nOrgNum" type="xsd:integer" minOccurs="0"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
    <xsd:element name="sCASName" type="xsd:string" minOccurs="0"/>
    <xsd:element name="sIUPACName" type="xsd:string" minOccurs="0">
      <xsd:annotation>
        <xsd:appinfo>IUPAC name, string</xsd:appinfo>
        <xsd:documentation>International Union of Physics and Applied Chemistry
name</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sCommonName" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">
      <xsd:annotation>
        <xsd:appinfo>Common name, string</xsd:appinfo>
        <xsd:documentation>Common name</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sFormulaMolec" type="xsd:string" minOccurs="0">
      <xsd:annotation>
        <xsd:appinfo>Molecular formula, string</xsd:appinfo>
        <xsd:documentation>Chemical molecular formula</xsd:documentation>
      </xsd:annotation>
    </xsd:element>
    <xsd:element name="sSmiles" type="xsd:string" minOccurs="0"
maxOccurs="unbounded">
      <xsd:annotation>

```

```

<xsd:appinfo>SMILES notation, string</xsd:appinfo>
<xsd:documentation>SMILES notation</xsd:documentation>
</xsd:annotation>
</xsd:element>
<xsd:element ref="Sample" minOccurs="0" maxOccurs="unbounded"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--

-->
<xsd:element name="Sample">
<xsd:annotation>
<xsd:documentation>sample</xsd:documentation>
</xsd:annotation>
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nSampleNm" type="xsd:integer"/>
<xsd:element name="eSource" type="eSampleSource" minOccurs="0"/>
<xsd:element name="eStatus" type="eSampleStatus" minOccurs="0"/>
<xsd:element name="purity" minOccurs="0" maxOccurs="unbounded">
<xsd:annotation>
<xsd:documentation>Purity of the sample</xsd:documentation>
</xsd:annotation>
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nStep" type="xsd:integer"/>
<xsd:element name="ePurifMethod" type="ePurifMethod" minOccurs="0"
maxOccurs="unbounded"/>
<xsd:element name="sPurifMethod" type="xsd:string" minOccurs="0"
maxOccurs="unbounded"/>
<xsd:sequence minOccurs="0">
<xsd:element name="nPurityMol" type="xsd:float">
<xsd:annotation>
<xsd:documentation>purity value in mole percent</xsd:documentation>
</xsd:annotation>
</xsd:element>
<xsd:element name="nPurityMolDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:sequence minOccurs="0">
<xsd:element name="nPurityMass" type="xsd:float">
<xsd:annotation>
<xsd:documentation>purity value in mass percent</xsd:documentation>

```

```

        </xsd:annotation>
    </xsd:element>
    <xsd:element name="nPurityMassDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:sequence minOccurs="0">
    <xsd:element name="nPurityVol" type="xsd:float">
        <xsd:annotation>
            <xsd:documentation>purity value in volume
percent</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="nPurityVolDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:sequence minOccurs="0">
    <xsd:element name="nWaterMassPerCent" type="xsd:float">
        <xsd:annotation>
            <xsd:documentation>mass per cent of water</xsd:documentation>
        </xsd:annotation>
    </xsd:element>
    <xsd:element name="nWaterMassPerCentDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:element name="eAnalMeth" type="ePurityAnalMethod" minOccurs="0"
maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:documentation>Analytical method used to determine
purity</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="sAnalMeth" type="xsd:string" minOccurs="0"
maxOccurs="unbounded"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="PureOrMixtureData">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="Component" maxOccurs="unbounded">

```

```

<xsd:complexType>
  <xsd:sequence>
    <xsd:element ref="RegNum"/>
    <xsd:element name="nSampleNm" type="xsd:int" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="eExpPurpose" type="eExpPurpose" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation>Purpose of measurement</xsd:documentation>
  </xsd:annotation>
</xsd:element>
<xsd:element name="sCompiler" type="xsd:string" minOccurs="0"/>
<xsd:element name="sContributor" type="xsd:string" minOccurs="0"/>
<xsd:element name="dateDateAdded" minOccurs="0"/>
<xsd:element name="Property" maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nPropNumber" type="xsd:integer"/>
      <xsd:element name="Property-MethodID">
        <xsd:annotation>
          <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
        </xsd:annotation>
      </xsd:element>
    </xsd:sequence>
    <xsd:element name="PropertyGroup">
      <xsd:complexType>
        <xsd:choice>
          <xsd:element name="Criticals">
            <xsd:complexType>
              <xsd:sequence>
                <xsd:element name="ePropName">
                  <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                      <xsd:enumeration value="Critical temperature, K"/>
                      <xsd:enumeration value="Critical pressure, kPa"/>
                      <xsd:enumeration value="Critical density, kg/m3"/>
                      <xsd:enumeration value="Critical molar volume, m3/mol"/>
                      <xsd:enumeration value="Critical specific volume, m3/kg"/>
                      <xsd:enumeration value="Critical compressibility"/>
                      <xsd:enumeration value="Lower consolute temperature,
K"/>

```

```

        <xsd:enumeration value="Upper consolute temperature,
K"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>
    <xsd:choice>
        <xsd:element name="eMethodName">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Visual observation in an
unstirred cell"/>
                    <xsd:enumeration value="Visual observation in a stirred
cell"/>
                    <xsd:enumeration value="DSC/DTA"/>
                    <xsd:enumeration value="Derived from PVT data"/>
                    <xsd:enumeration value="Extrapolated vapor pressure"/>
                    <xsd:enumeration value="Rectilinear diameter"/>
                    <xsd:enumeration value="Appearance of two phases"/>
                    <xsd:enumeration value="Disappearance of two phases"/>
                    <xsd:enumeration value="Direct measurement"/>
                    <xsd:enumeration value="Other"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:element name="sMethodName" type="xsd:string"/>
        <xsd:element ref="CriticalEvaluation"/>
        <xsd:element ref="Prediction"/>
    </xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="VaporPBoilingTAzeotropTandP">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePropName">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Vapor or Sublimation pressure,
kPa"/>
                        <xsd:enumeration value="Normal boiling temperature, K"/>
                        <xsd:enumeration value="Boiling temperature at pressure P,
K"/>
                        <xsd:enumeration value="Azeotropic pressure, kPa"/>

```

```

        <xsd:enumeration value="Azeotropic temperature, K"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
    <xsd:element name="eMethodName">
        <xsd:simpleType>
            <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Manometric method"/>
                <xsd:enumeration value="Closed cell (Static) method"/>
                <xsd:enumeration value="Diaphragm manometer"/>
                <xsd:enumeration value="Inclined piston gauge"/>
                <xsd:enumeration value="Isochoric PVT apparatus"/>
                <xsd:enumeration value="Isoteniscope"/>
                <xsd:enumeration value="Knudsen effusion method"/>
                <xsd:enumeration value="Distillation"/>
                <xsd:enumeration value="Ebulliometric method
(Recirculating still)"/>
                <xsd:enumeration value="Twin ebulliometer"/>
                <xsd:enumeration value="Transpiration method"/>
                <xsd:enumeration value="Rate of evaporation"/>
                <xsd:enumeration value="By X=Y"/>
                <xsd:enumeration value="By P(X) extreme"/>
                <xsd:enumeration value="By T(X) extreme"/>
                <xsd:enumeration value="Other"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>
    <xsd:element name="sMethodName" type="xsd:string"/>
    <xsd:element ref="CriticalEvaluation"/>
    <xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="PhaseTransition">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePropName">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Triple point temperature, K"/>
                        <xsd:enumeration value="Triple point pressure, kPa"/>

```

```

<xsd:enumeration value="Normal melting temperature, K"/>
<xsd:enumeration value="Enthalpy of transition or fusion,
kJ/mol"/>

sublimation, kJ/mol"/>
temperature, K"/>
pressure, kPa"/>
temperature, K"/>
temperature, K"/>
analysis"/>
calorimetry"/>
constant"/>
analysis"/>
precise ebulliometry"/>
a dilute solution"/>

<xsd:enumeration value="Cryoscopic constant, 1/K"/>
<xsd:enumeration value="Enthalpy of vaporization or
Quadruple (quintuple) point
Quadruple (quintuple) point
Solid-liquid equilibrium
Liquid-liquid equilibrium
Eutectic temperature, K"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
<xsd:element name="eMethodName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Visual observation"/>
<xsd:enumeration value="Heating/Cooling curves"/>
<xsd:enumeration value="DSC/DTA"/>
<xsd:enumeration value="Adiabatic calorimetry"/>
<xsd:enumeration value="Large-sample thermal
Drop calorimetry"/>
<xsd:enumeration value="Drop ice or diphenyl ether
Obtained from cryoscopic
Derived from phase diagram
Static calorimetry"/>
<xsd:enumeration value="Flow calorimetry"/>
<xsd:enumeration value="Derived by Second law"/>
<xsd:enumeration value="Derived by Second law from
Depression of a freezing point of
Other"/>

```

```

        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
<xsd:element ref="Prediction"/>
<xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="CompositionAtPhaseEquilibrium">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePropName">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Azeotropic composition: mole
fraction"/>
                        <xsd:enumeration value="Azeotropic composition: mass
fraction"/>
                        <xsd:enumeration value="Eutectic composition: volume
fraction"/>
                        <xsd:enumeration value="Eutectic composition: mole
fraction"/>
                        <xsd:enumeration value="Eutectic composition: mass
fraction"/>
                        <xsd:enumeration value="Lower consolute composition:
volume fraction"/>
                        <xsd:enumeration value="Lower consolute composition:
mole fraction"/>
                        <xsd:enumeration value="Lower consolute composition:
mass fraction"/>
                        <xsd:enumeration value="Mass per volume of solution,
kg/m3"/>
                        <xsd:enumeration value="Mass ratio to solvent"/>
                        <xsd:enumeration value="Molar concentration, mol/kg"/>
                        <xsd:enumeration value="Molar concentration, mol/dm3"/>
                        <xsd:enumeration value="Mole fraction"/>
                        <xsd:enumeration value="Mole fraction in LLG critical
state"/>
                        <xsd:enumeration value="Mole ratio to solvent"/>
                        <xsd:enumeration value="Moles per mass of solution,
mol/kg"/>

```

```

<xsd:enumeration value="Upper consolute composition:
volume fraction"/>

<xsd:enumeration value="Upper consolute composition:
mole fraction"/>

<xsd:enumeration value="Upper consolute composition:
mass fraction"/>

<xsd:enumeration value="Volume fraction"/>
<xsd:enumeration value="Volume ratio to solvent"/>
<xsd:enumeration value="Mass fraction"/>
<xsd:enumeration value="Mass fraction in LLG critical
state"/>

<xsd:enumeration value="Henry's Law constant for mole
fraction, kPa"/>
<xsd:enumeration value="Henry's Law constant (molarity),
kPa kg/mol"/>
<xsd:enumeration value="Henry's Law constant (molarity),
kPa l/mol"/>

<xsd:enumeration value="Bunsen coefficient"/>
<xsd:enumeration value="Ostwald coefficient"/>
<xsd:enumeration value="Partial pressure, kPa"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
<xsd:element name="eMethodName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="By X=Y"/>
<xsd:enumeration value="By T or P extreme"/>
<xsd:enumeration value="Chromatography"/>
<xsd:enumeration value="Spectrophotometry"/>
<xsd:enumeration value="Determined by refractive index
and/or density"/>
<xsd:enumeration value="Calculated by Gibbs-Duhem
equation"/>
<xsd:enumeration value="Titration method"/>
<xsd:enumeration value="Static method"/>
<xsd:enumeration value="Dynamic method"/>
<xsd:enumeration value="Phase equilibration"/>
<xsd:enumeration value="Derived from phase diagram
analysis"/>
<xsd:enumeration value="Appearance of two phases"/>
<xsd:enumeration value="Disappearance of two phases"/>

```

```

        <xsd:enumeration value="Photoacoustic method"/>
        <xsd:enumeration value="Other"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
<xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="ActivityFugacityOsmoticProp">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="ePropName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Activity"/>
<xsd:enumeration value="Activity coefficient"/>
<xsd:enumeration value="Fugacity, kPa"/>
<xsd:enumeration value="Fugacity coefficient"/>
<xsd:enumeration value="Osmotic pressure, kPa"/>
<xsd:enumeration value="Osmotic coefficient"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
<xsd:element name="eMethodName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Chromatography"/>
<xsd:enumeration value="Spectroscopy"/>
<xsd:enumeration value="Mass-spectrometry"/>
<xsd:enumeration value="NMR spectrometry"/>
<xsd:enumeration value="Static method"/>
<xsd:enumeration value="Isopiestic method"/>
<xsd:enumeration value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>

```

```

<xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="VolumetricProp">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="ePropName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Specific density, kg/m3"/>
<xsd:enumeration value="Specific volume, m3/kg"/>
<xsd:enumeration value="Molar density, mol/m3"/>
<xsd:enumeration value="Molar volume, m3/mol"/>
<xsd:enumeration value="2nd virial coefficient, m3/mol"/>
<xsd:enumeration value="2nd acoustic virial coefficient,
m3/mol"/>
<xsd:enumeration value="3rd virial coefficient, m6/mol2"/>
<xsd:enumeration value="3rd acoustic virial coefficient,
m6/mol2"/>
<xsd:enumeration value="3rd interaction virial coefficient
C112, m6/mol2"/>
<xsd:enumeration value="3rd interaction virial coefficient
C122, m6/mol2"/>
<xsd:enumeration value="Excess virial coefficient,
m3/mol"/>
<xsd:enumeration value="Interaction virial coefficient,
m3/mol"/>
<xsd:enumeration value="Excess volume, m3/mol"/>
<xsd:enumeration value="Partial molar volume, m3/mol"/>
<xsd:enumeration value="Relative partial molar volume,
m3/mol"/>
<xsd:enumeration value="Apparent molar volume,
m3/mol"/>
<xsd:enumeration value="Adiabatic compressibility,
1/kPa"/>
<xsd:enumeration value="Isothermal compressibility,
1/kPa"/>
<xsd:enumeration value="Coefficient of expansion, 1/K"/>
<xsd:enumeration value="Compressibility factor"/>
<xsd:enumeration value="Thermal pressure coefficient,
kPa/K"/>

```

```

        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
<xsd:choice>
    <xsd:element name="eMethodName">
        <xsd:simpleType>
            <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Pycnometric method"/>
                <xsd:enumeration value="Buoyancy method"/>
                <xsd:enumeration value="Vibrating tube method"/>
                <xsd:enumeration value="Isochoric PVT measurement"/>
                <xsd:enumeration value="Other PVT measurement"/>
                <xsd:enumeration value="Burnett expansion technique"/>
                <xsd:enumeration value="Constant-volume piesometry"/>
                <xsd:enumeration value="Direct dilatometry"/>
                <xsd:enumeration value="Derived analytically"/>
                <xsd:enumeration value="Derived graphically"/>
                <xsd:enumeration value="Calculated with densities of this
investigation"/>
                <xsd:enumeration value="Calculated with a solvent density
reported elsewhere"/>
                    <xsd:enumeration value="Other"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>
    <xsd:element name="sMethodName" type="xsd:string"/>
    <xsd:element ref="CriticalEvaluation"/>
    <xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="HeatCapacityAndDerivedProp">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePropName">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Heat capacity at constant pressure
Cp, J/K/mol"/>
                        <xsd:enumeration value="Heat capacity at vapor saturation
pressure Csat, J/K/mol"/>

```

```

        <xsd:enumeration value="Heat capacity at constant volume
Cv, J/K/mol"/>
        <xsd:enumeration value="Heat capacity at constant pressure
Cp per unit mass, J/K/kg"/>
            <xsd:enumeration value="Heat capacity at constant pressure
Cp per unit volume, J/K/m3"/>
                <xsd:enumeration value="Heat capacity at constant volume
Cv per unit mass, J/K/kg"/>
                <xsd:enumeration value="Heat capacity at constant volume
Cv per unit volume, J/K/m3"/>
                    <xsd:enumeration value="Heat capacity ratio Cp/Cv"/>
                    <xsd:enumeration value="Entropy, J/K/mol"/>
                    <xsd:enumeration value="Enthalpy, kJ/mol"/>
                    <xsd:enumeration value="Enthalpy function {H(T)-H(0)}/T,
J/K/mol"/>
                    <xsd:enumeration value="Gibbs energy function {G(T)-
H(0)}/T, J/K/mol"/>
                    <xsd:enumeration value="Gibbs energy, kJ/mol"/>
                    <xsd:enumeration value="Helmholtz energy, kJ/mol"/>
                    <xsd:enumeration value="Internal energy, kJ/mol"/>
                    <xsd:enumeration value="Joule-Thomson coefficient,
K/kPa"/>
                    <xsd:enumeration value="Pressure coefficient of enthalpy,
J/mol/kPa"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:choice>
            <xsd:element name="eMethodName">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Vacuum adiabatic calorimetry"/>
                        <xsd:enumeration value="Small (less than 1 g) adiabatic
calorimetry"/>
                        <xsd:enumeration value="Flow calorimetry"/>
                        <xsd:enumeration value="Large sample (1 g) DSC"/>
                        <xsd:enumeration value="Small sample (50 mg) DSC"/>
                        <xsd:enumeration value="Drop calorimetry"/>
                        <xsd:enumeration value="Drop ice or diphenyl ether
calorimetry"/>
                        <xsd:enumeration value="Open cup calorimetry"/>
                        <xsd:enumeration value="Closed cup calorimetry"/>
                        <xsd:enumeration value="Differential flow calorimetry"/>

```

```

        <xsd:enumeration value="Extra sensitive DSC"/>
        <xsd:enumeration value="Twin closed calorimetry"/>
        <xsd:enumeration value="Derived from speed of sound"/>
        <xsd:enumeration value="Derived from equation of
state"/>
            <xsd:enumeration value="Expansion technique"/>
                <xsd:enumeration value="Other"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
    <xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="ExcessPartialApparentEnergyProp">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="ePropName">
                <xsd:simpleType>
                    <xsd:restriction base="xsd:string">
                        <xsd:enumeration value="Apparent enthalpy, kJ/mol"/>
                        <xsd:enumeration value="Apparent entropy, J/K/mol"/>
                        <xsd:enumeration value="Apparent Gibbs energy, kJ/mol"/>
                        <xsd:enumeration value="Apparent molar heat capacity,
J/K/mol"/>
                        <xsd:enumeration value="Enthalpy of mixing with a binary
solvent, kJ/mol"/>
                        <xsd:enumeration value="Excess enthalpy, kJ/mol"/>
                        <xsd:enumeration value="Enthalpy of mixing with binary
solvent, kJ/mol"/>
                        <xsd:enumeration value="Excess entropy, J/K/mol"/>
                        <xsd:enumeration value="Excess Gibbs energy, kJ/mol"/>
                        <xsd:enumeration value="Excess heat capacity, J/K/mol"/>
                        <xsd:enumeration value="Partial molar enthalpy, kJ/mol"/>
                        <xsd:enumeration value="Partial molar entropy, J/K/mol"/>
                        <xsd:enumeration value="Partial molar Gibbs energy,
kJ/mol"/>
                        <xsd:enumeration value="Partial molar heat capacity,
J/K/mol"/>
                    </xsd:restriction>
                </xsd:simpleType>
            </xsd:element>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>

```

```

        <xsd:enumeration value="Relative partial molar enthalpy,
kJ/mol"/>

        <xsd:enumeration value="Relative partial molar entropy,
J/K/mol"/>

        <xsd:enumeration value="Relative partial molar Gibbs
energy, kJ/mol"/>

        <xsd:enumeration value="Relative partial molar heat
capacity, J/K/mol"/>

        <xsd:enumeration value="Standard state enthalpy, kJ/mol"/>
        <xsd:enumeration value="Standard state entropy, J/K/mol"/>
        <xsd:enumeration value="Standard state Gibbs energy,
kJ/mol"/>

        <xsd:enumeration value="Standard state heat capacity,
J/K/mol"/>

        <xsd:enumeration value=""/>
        </xsd:restriction>
        </xsd:simpleType>
</xsd:element>
<xsd:choice>
    <xsd:element name="eMethodName">
        <xsd:simpleType>
            <xsd:restriction base="xsd:string">
                <xsd:enumeration value="Vacuum adiabatic calorimetry"/>
                <xsd:enumeration value="Small (less than 1 g) adiabatic
calorimetry"/>
                <xsd:enumeration value="Flow calorimetry"/>
                <xsd:enumeration value="Differential flow calorimetry"/>
                <xsd:enumeration value="Calvet calorimetry"/>
                <xsd:enumeration value="Large sample (1 g) DSC"/>
                <xsd:enumeration value="Small sample (50 mg) DSC"/>
                <xsd:enumeration value="Extra sensitive DSC"/>
                <xsd:enumeration value="Twin closed calorimetry"/>
                <xsd:enumeration value="Other"/>
            </xsd:restriction>
        </xsd:simpleType>
    </xsd:element>
    <xsd:element name="sMethodName" type="xsd:string"/>
    <xsd:element ref="CriticalEvaluation"/>
    <xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>

```

```

<xsd:element name="TransportProp">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="ePropName">
        <xsd:simpleType>
          <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Viscosity, Pa*s"/>
            <xsd:enumeration value="Kinematic viscosity, m2/s"/>
            <xsd:enumeration value="Fluidity, 1/Pa/s"/>
            <xsd:enumeration value="Thermal conductivity, W/m/K"/>
            <xsd:enumeration value="Thermal diffusivity, m2/s"/>
            <xsd:enumeration value="Binary diffusion coefficient, 1e-9
m2/s"/>
            <xsd:enumeration value="Self diffusion coefficient, 1e-9
m2/s"/>
            <xsd:enumeration value="Tracer diffusion coefficient, 1e-9
m2/s"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
    <xsd:choice>
      <xsd:element name="eMethodName">
        <xsd:simpleType>
          <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Capillary tube (Ostwald;
Ubellohde) method"/>
            <xsd:enumeration value="Cone and plate viscometry"/>
            <xsd:enumeration value="Concentric cylinders
viscometry"/>
            <xsd:enumeration value="Falling or rolling sphere
viscometry"/>
            <xsd:enumeration value="Oscillating disk viscometry"/>
            <xsd:enumeration value="Vibrating wire viscometry"/>
            <xsd:enumeration value="Parallel plate method"/>
            <xsd:enumeration value="Coaxial cylinder method"/>
            <xsd:enumeration value="Hot wire method"/>
            <xsd:enumeration value="Optical interferometry"/>
            <xsd:enumeration value="Dispersion"/>
            <xsd:enumeration value="Diaphragm Cell"/>
            <xsd:enumeration value="Open capillary"/>
            <xsd:enumeration value="Closed capillary"/>
            <xsd:enumeration value="Taylor dispersion method"/>
            <xsd:enumeration value="NMR spin-echo technique"/>

```

```

        <xsd:enumeration value="Other"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
<xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="RefractionSurfaceTensionSoundSpeed">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="ePropName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Refractive index (Na D-line)"/>
<xsd:enumeration value="Refractive index (other
wavelength)"/>
<xsd:enumeration value="Surface tension liquid-gas, N/m"/>
<xsd:enumeration value="Interfacial tension, N/m"/>
<xsd:enumeration value="Speed of sound, m/s"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
<xsd:element name="eMethodName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Standard Abbe refractometry"/>
<xsd:enumeration value="Precision Abbe refractometry"/>
<xsd:enumeration value="Dipping refractometry
(monochromatic)"/>
<xsd:enumeration value="Interferometer"/>
<xsd:enumeration value="Capillary rise"/>
<xsd:enumeration value="Drop weight"/>
<xsd:enumeration value="Drop volume"/>
<xsd:enumeration value="Maximal bubble pressure"/>
<xsd:enumeration value="Pendant drop shape"/>
<xsd:enumeration value="Ring tensiometer"/>
<xsd:enumeration value="Linear variable-path acoustic
interferometer"/>

```

```

        <xsd:enumeration value="Sing-around technique in a
fixed-path interferometer"/>
            <xsd:enumeration value="Annular interferometer"/>
            <xsd:enumeration value="Pulse-echo method"/>
            <xsd:enumeration value="Spherical resonator"/>
            <xsd:enumeration value="Light diffraction method"/>
            <xsd:enumeration value="Other"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
    <xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:choice>
</xsd:complexType>
</xsd:element>
<xsd:element ref="RegNum" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="PropPhaseID" minOccurs="0">
    <xsd:annotation>
        <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
    </xsd:annotation>
<xsd:complexType>
    <xsd:sequence>
        <xsd:element name="ePropPhase" type="ePhaseName"/>
        <xsd:element ref="RegNum" minOccurs="0">
            <xsd:annotation>
                <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
            </xsd:annotation>
        </xsd:element>
        <xsd:sequence>
            <xsd:element name="ePresentation" type="ePresentation"/>
            <xsd:element name="eRefStateType" type="eRefStateType" minOccurs="0"/>
        </xsd:sequence>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>

```

```

<xsd:sequence minOccurs="0">
  <xsd:element name="nRefTemp" type="xsd:float"/>
  <xsd:element name="nRefTempDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:sequence minOccurs="0">
  <xsd:element name="nRefPressure" type="xsd:float"/>
  <xsd:element name="nRefPressureDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:element name="RefPhaseID" minOccurs="0">
  <xsd:annotation>
    <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
  </xsd:annotation>
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="eRefPhase" type="ePhaseName"/>
      <xsd:element ref="RegNum" minOccurs="0"/>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<xsd:element ref="Solvent" minOccurs="0"/>
<xsd:element name="eStandardState" minOccurs="0">
  <xsd:simpleType>
    <xsd:restriction base="xsd:string">
      <xsd:enumeration value="Pure compound"/>
      <xsd:enumeration value="Hypothetical pure solute"/>
      <xsd:enumeration value="Hypothetical unit molality solute"/>
      <xsd:enumeration value="Hypothetical unit molarity solute"/>
      <xsd:enumeration value="Infinite dilution solute"/>
    </xsd:restriction>
  </xsd:simpleType>
</xsd:element>
<xsd:element ref="CombinedUncertainty" minOccurs="0"
maxOccurs="unbounded"/>
  <xsd:element name="PropUncertainty" type="PropVarUncertaintyType"
minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="PropRepeatability" type="PropVarRepeatabilityType"
minOccurs="0"/>
      <xsd:element name="PropDeviceSpec" type="PropVarDeviceSpecType"
minOccurs="0"/>
        <xsd:element ref="CurveDev" minOccurs="0" maxOccurs="unbounded"/>
      </xsd:sequence>
    </xsd:complexType>

```

```

</xsd:element>
<xsd:element name="PhaseID" maxOccurs="unbounded">
  <xsd:annotation>
    <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
  </xsd:annotation>
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="ePhase" type="ePhaseName"/>
      <xsd:element ref="RegNum" minOccurs="0"/>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<xsd:element name="Constraint" minOccurs="0" maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nConstraintNumber" type="xsd:integer"
minOccurs="0"/>
      <xsd:element name="ConstraintID">
        <xsd:annotation>
          <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
        </xsd:annotation>
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="ConstraintType" type="ConstraintVariableType"/>
            <xsd:element ref="RegNum" minOccurs="0"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="ConstraintPhaseID" minOccurs="0">
        <xsd:annotation>
          <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
        </xsd:annotation>
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="eConstraintPhase" type="ePhaseName"/>
            <xsd:element ref="RegNum" minOccurs="0"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element ref="Solvent" minOccurs="0"/>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>

```

```

<xsd:element name="nConstraintValue" type="xsd:float"/>
<xsd:element name="nConstrDigits" type="xsd:integer"/>
<xsd:element name="ConstrUncertainty" type="ConstrUncertaintyType"
minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="ConstrRepeatability" type="ConstrRepeatabilityType"
minOccurs="0"/>
        <xsd:element name="ConstrDeviceSpec" type="ConstrDeviceSpecType"
minOccurs="0"/>
            </xsd:sequence>
        </xsd:complexType>
    </xsd:element>
<xsd:element name="Variable" minOccurs="0" maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nVarNumber" type="xsd:integer"/>
            <xsd:element name="VariableID">
                <xsd:annotation>
                    <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
                </xsd:annotation>
            </xsd:complexType>
            <xsd:sequence>
                <xsd:element name="VariableType" type="ConstraintVariableType"/>
                <xsd:element ref="RegNum" minOccurs="0"/>
            </xsd:sequence>
        </xsd:complexType>
    </xsd:element>
<xsd:element name="VarPhaseID" minOccurs="0">
    <xsd:annotation>
        <xsd:documentation> CASRN is necessary for mixtures
only</xsd:documentation>
    </xsd:annotation>
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="eVarPhase" type="ePhaseName"/>
            <xsd:element ref="RegNum" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>

```

```

<xsd:element name="VarRepeatability" type="PropVarRepeatabilityType"
minOccurs="0"/>
    <xsd:element name="VarDeviceSpec" type="PropVarDeviceSpecType"
minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element ref="NumValues" minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element ref="Equation" minOccurs="0" maxOccurs="unbounded"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="ReactionData">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="Participant" maxOccurs="unbounded">
                <xsd:complexType>
                    <xsd:sequence>
                        <xsd:element ref="RegNum"/>
                        <xsd:element name="nSampleNm" type="xsd:int" minOccurs="0"/>
                        <xsd:element name="nStoichiometricCoef" type="xsd:float"/>
                        <xsd:element name="ePhase" type="ePhaseName"/>
                        <xsd:element name="eCompositionRepresentation" minOccurs="0">
                            <xsd:annotation>
                                <xsd:documentation>Only for reactions with the initial state
change</xsd:documentation>
                            </xsd:annotation>
                            <xsd:simpleType>
                                <xsd:restriction base="xsd:string">
                                    <xsd:enumeration value="Mole ratio of solvent to participant"/>
                                    <xsd:enumeration value="Molality (moles of participant per kilogram of
solvent)"/>
                                    <xsd:enumeration value="Moles of participant per kilogram of solution"/>
                                    <xsd:enumeration value="Molarity (moles of participant per liter of
solution)"/>
                                    <xsd:enumeration value="Mole ratio (moles of participant per mole of
solvent)"/>
                                    <xsd:enumeration value="Mass ratio (mass of participant per mass of
solvent)"/>

```

```

        <xsd:enumeration value="Volume ratio (volume of participant per volume
of solvent)"/>
            <xsd:enumeration value="Mass of participant (kg) per volume of solution
(m^-3)"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
    <xsd:element name="nNumericalComposition" type="xsd:float"
minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<xsd:element name="eExpPurpose" type="eExpPurpose" minOccurs="0">
    <xsd:annotation>
        <xsd:documentation>Purpose of measurement</xsd:documentation>
    </xsd:annotation>
</xsd:element>
<xsd:element name="sCompiler" type="xsd:string" minOccurs="0"/>
<xsd:element name="sContributor" type="xsd:string" minOccurs="0"/>
<xsd:element name="dateDateAdded" minOccurs="0"/>
<xsd:element name="eReactionType">
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Combustion with oxygen"/>
            <xsd:enumeration value="Addition of various compounds to unsaturated
compounds"/>
            <xsd:enumeration value="Addition of water to a liquid or solid to produce a
hydrate"/>
            <xsd:enumeration value="Atomization (or formation from atoms)"/>
            <xsd:enumeration value="Combustion with other elements or compounds"/>
            <xsd:enumeration value="Esterification"/>
            <xsd:enumeration value="Exchange of alkyl groups"/>
            <xsd:enumeration value="Exchange of hydrogen (atoms) with other groups"/>
            <xsd:enumeration value="Formation of a compound from elements in their
stable state"/>
            <xsd:enumeration value="Halogenation (addition of or replacement by a
halogen)"/>
            <xsd:enumeration value="Hydrogenation (addition of H2 to unsaturated
compounds)"/>
            <xsd:enumeration value="Hydrohalogenation"/>
            <xsd:enumeration value="Hydrolysis of ions"/>
            <xsd:enumeration value="Other reactions with water"/>
            <xsd:enumeration value="Ion exchange"/>

```

```

<xsd:enumeration value="Neutralization (reaction of an acid with a base)"/>
<xsd:enumeration value="Oxidation with oxidizing agents other than
oxygen"/>
<xsd:enumeration value="Oxidation with oxygen (not complete)"/>
<xsd:enumeration value="Polymerization (all other types)"/>
<xsd:enumeration value="Homonuclear dimerization"/>
<xsd:enumeration value="Solvolyis (solvents other than water)"/>
<xsd:enumeration value="Stereoisomerism"/>
<xsd:enumeration value="Structural isomerization"/>
<xsd:enumeration value="Other reactions"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="Property" maxOccurs="unbounded">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nPropNumber" type="xsd:integer"/>
<xsd:element name="Property-MethodID">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="PropertyGroup">
<xsd:complexType>
<xsd:choice>
<xsd:element name="EnthalpyInternalEnergyOfReaction">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="ePropName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Enthalpy of reaction, kJ/mol"/>
<xsd:enumeration value="Internal energy of reaction (mass
basis), J/g"/>
<xsd:enumeration value="Internal energy of reaction (mole
basis), kJ/mol"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
<xsd:element name="eMethodName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Static bomb calorimetry"/>
<xsd:enumeration value="Rotating bomb calorimetry"/>

```

```

        <xsd:enumeration value="Micro-bomb calorimetry"/>
        <xsd:enumeration value="Flame calorimetry"/>
        <xsd:enumeration value="Other"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
<xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="ReactionEquilibriumProp">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="ePropName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Thermodynamic equilibrium
constant"/>
        <xsd:enumeration value="Apparent equilibrium constant in
terms of molality, (mol/kg)n"/>
        <xsd:enumeration value="Apparent equilibrium constant in
terms of molarity, (mol/dm3)n"/>
        <xsd:enumeration value="Apparent equilibrium constant in
terms of pressure, kPan"/>
        <xsd:enumeration value="Apparent equilibrium constant in
terms of mole fraction X"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:choice>
<xsd:element name="eMethodName">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Static equilibration"/>
<xsd:enumeration value="Dynamic equilibration"/>
<xsd:enumeration value="Chromatography"/>
<xsd:enumeration value="IR spectrometry"/>
<xsd:enumeration value="UV spectroscopy"/>
<xsd:enumeration value="NMR spectrometry"/>
<xsd:enumeration value="Titration"/>

```

```

        <xsd:enumeration value="Other"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sMethodName" type="xsd:string"/>
<xsd:element ref="CriticalEvaluation"/>
<xsd:element ref="Prediction"/>
</xsd:choice>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:choice>
</xsd:complexType>
</xsd:element>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Solvent" minOccurs="0">
<xsd:complexType>
<xsd:sequence>
<xsd:element ref="RegNum"/>
<xsd:element name="ePhase" type="ePhaseName"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Catalyst" minOccurs="0">
<xsd:complexType>
<xsd:sequence>
<xsd:element ref="RegNum"/>
<xsd:element name="ePhase" type="ePhaseName" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="eStandardState" minOccurs="0">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Pure compound"/>
<xsd:enumeration value="Hypothetical pure solute"/>
<xsd:enumeration value="Hypothetical unit molality solute"/>
<xsd:enumeration value="Hypothetical unit molarity solute"/>
<xsd:enumeration value="Infinite dilution solute"/>
</xsd:restriction>
</xsd:simpleType>

```

```

</xsd:element>
<xsd:sequence minOccurs="0">
  <xsd:element name="nTemperature-K" type="xsd:float">
    <xsd:annotation>
      <xsd:documentation> Only for reactions with the initial state
change</xsd:documentation>
    </xsd:annotation>
  </xsd:element>
  <xsd:element name="nTemperatureDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:sequence minOccurs="0">
  <xsd:element name="nPressure-kPa" type="xsd:float">
    <xsd:annotation>
      <xsd:documentation> Only for reactions with the initial state
change</xsd:documentation>
    </xsd:annotation>
  </xsd:element>
  <xsd:element name="nPressureDigits" type="xsd:integer"/>
</xsd:sequence>
<xsd:element ref="CombinedUncertainty" minOccurs="0"
maxOccurs="unbounded"/>
  <xsd:element name="PropUncertainty" type="PropVarUncertaintyType"
minOccurs="0" maxOccurs="unbounded"/>
  <xsd:element name="PropRepeatability" type="PropVarRepeatabilityType"
minOccurs="0"/>
  <xsd:element name="PropDeviceSpec" type="PropVarDeviceSpecType"
minOccurs="0"/>
    <xsd:element ref="CurveDev" minOccurs="0" maxOccurs="unbounded"/>
  </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Constraint" minOccurs="0" maxOccurs="unbounded">
  <xsd:annotation>
    <xsd:documentation>Only for reactions in equilibrium</xsd:documentation>
  </xsd:annotation>
</xsd:complexType>
<xsd:sequence>
  <xsd:element name="nConstraintNumber" type="xsd:integer"
minOccurs="0"/>
  <xsd:element name="ConstraintID">
    <xsd:complexType>
      <xsd:sequence>
        <xsd:element name="ConstraintType" type="ConstraintVariableType"/>

```

```

        <xsd:element ref="RegNum" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="nConstraintValue" type="xsd:float"/>
<xsd:element name="nConstrDigits" type="xsd:integer"/>
<xsd:element name="ConstrUncertainty" type="ConstrUncertaintyType"
minOccurs="0" maxOccurs="unbounded"/>
    <xsd:element name="ConstrRepeatability" type="ConstrRepeatabilityType"
minOccurs="0"/>
        <xsd:element name="ConstrDeviceSpec" type="ConstrDeviceSpecType"
minOccurs="0"/>
            </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Variable" minOccurs="0" maxOccurs="unbounded">
    <xsd:annotation>
        <xsd:documentation>Only for reactions in equilibrium</xsd:documentation>
    </xsd:annotation>
<xsd:complexType>
    <xsd:sequence>
        <xsd:element name="nVarNumber" type="xsd:integer"/>
        <xsd:element name="VariableID">
            <xsd:complexType>
                <xsd:sequence>
                    <xsd:element name="VariableType" type="ConstraintVariableType"/>
                    <xsd:element ref="RegNum" minOccurs="0"/>
                </xsd:sequence>
            </xsd:complexType>
        </xsd:element>
        <xsd:element name="VarUncertainty" type="PropVarUncertaintyType"
minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element name="VarRepeatability" type="PropVarRepeatabilityType"
minOccurs="0"/>
                <xsd:element name="VarDeviceSpec" type="PropVarDeviceSpecType"
minOccurs="0"/>
                    </xsd:sequence>
                </xsd:complexType>
            </xsd:element>
            <xsd:element ref="NumValues" minOccurs="0" maxOccurs="unbounded"/>
            <xsd:element ref="Equation" minOccurs="0" maxOccurs="unbounded"/>
        </xsd:sequence>
    </xsd:complexType>

```

```

</xsd:element>
<!--

-->
<xsd:simpleType name="eSampleStatus">
  <xsd:annotation>
    <xsd:documentation>The sample status</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="unknown"/>
    <xsd:enumeration value="notDescribed"/>
    <xsd:enumeration value="previousPaper"/>
    <xsd:enumeration value="compilation"/>
  </xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="eSampleSource">
  <xsd:annotation>
    <xsd:documentation>Source(s) of the sample</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Commercial source"/>
    <xsd:enumeration value="Synthesized by the authors"/>
    <xsd:enumeration value="Synthesized by others"/>
    <xsd:enumeration value="Standard Reference Material (SRM)"/>
    <xsd:enumeration value="Isolated from a natural product"/>
    <xsd:enumeration value="Not stated in the document"/>
    <xsd:enumeration value="No sample used"/>
  </xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="ePurifMethod">
  <xsd:annotation>
    <xsd:documentation>Purification method(s) used to purify
sample</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Impurity adsorption"/>
    <xsd:enumeration value="Vacuum degasification"/>

```

```

<xsd:enumeration value="Chemical reagent treatment"/>
<xsd:enumeration value="Crystallization from melt"/>
<xsd:enumeration value="Crystallization from solution"/>
<xsd:enumeration value="Liquid chromatography"/>
<xsd:enumeration value="Dried with chemical reagent"/>
<xsd:enumeration value="Dried in a desiccator"/>
<xsd:enumeration value="Dried by oven heating"/>
<xsd:enumeration value="Dried by vacuum heating"/>
<xsd:enumeration value="De-gassed by freezing and melting in vacuum"/>
<xsd:enumeration value="De-gassed by boiling or ultrasonically"/>
<xsd:enumeration value="Fractional crystallization"/>
<xsd:enumeration value="Fractional distillation"/>
<xsd:enumeration value="Molecular sieve treatment"/>
<xsd:enumeration value="Unspecified"/>
<xsd:enumeration value="Preparative gas chromatography"/>
<xsd:enumeration value="Sublimation"/>
<xsd:enumeration value="Steam distillation"/>
<xsd:enumeration value="Solvent extraction"/>
<xsd:enumeration value="Salting out of solution"/>
<xsd:enumeration value="Zone refining"/>
<xsd:enumeration value="Other"/>
<xsd:enumeration value="None used"/>
</xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="ePurityAnalMethod">
  <xsd:annotation>
    <xsd:documentation>Analytical method used to measure
    purity.</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Chemical analysis"/>
    <xsd:enumeration value="Difference between bubble and dew points"/>
    <xsd:enumeration value="Density"/>
    <xsd:enumeration value="DSC"/>
    <xsd:enumeration value="Estimation"/>
    <xsd:enumeration value="Gas chromatography"/>
    <xsd:enumeration value="Fraction melting in an adiabatic calorimeter"/>
    <xsd:enumeration value="Mass spectrometry"/>
    <xsd:enumeration value="Not known"/>
    <xsd:enumeration value="Spectroscopy"/>
  </xsd:restriction>
</xsd:simpleType>

```

```

<xsd:enumeration value="Thermal analysis using temperature-time measurement"/>
<xsd:enumeration value="Acid-base titration"/>
<xsd:enumeration value="Mass loss on drying"/>
<xsd:enumeration value="HPLC"/>
<xsd:enumeration value="CO2 yield in combustion products"/>
<xsd:enumeration value="Other"/>
<xsd:enumeration value="Estimated by the compiler"/>
</xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="eExpPurpose">
<xsd:annotation>
  <xsd:documentation>Purpose of measurement</xsd:documentation>
</xsd:annotation>
<xsd:restriction base="xsd:string">
  <xsd:enumeration value="Principal objective of the work"/>
  <xsd:enumeration value="Secondary purpose (by-product of other objective)"/>
  <xsd:enumeration value="Determined for identification of a synthesized
compound"/>
</xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:simpleType name="ePhaseName">
<xsd:annotation>
  <xsd:documentation>Phase description</xsd:documentation>
</xsd:annotation>
<xsd:restriction base="xsd:string">
  <xsd:enumeration value="Crystal 4"/>
  <xsd:enumeration value="Crystal 3"/>
  <xsd:enumeration value="Crystal 2"/>
  <xsd:enumeration value="Crystal 1"/>
  <xsd:enumeration value="Crystal"/>
  <xsd:enumeration value="Crystal of unknown type"/>
  <xsd:enumeration value="Crystal of intercomponent compound 1"/>
  <xsd:enumeration value="Crystal of intercomponent compound 2"/>
  <xsd:enumeration value="Crystal of intercomponent compound 3"/>
  <xsd:enumeration value="Metastable crystal"/>
  <xsd:enumeration value="Glass"/>
  <xsd:enumeration value="Smectic liquid crystal"/>

```

```

<xsd:enumeration value="Nematic liquid crystal"/>
<xsd:enumeration value="Cholesteric liquid crystal"/>
<xsd:enumeration value="Liquid"/>
<xsd:enumeration value="Liquid mixture 1"/>
<xsd:enumeration value="Liquid mixture 2"/>
<xsd:enumeration value="Solution 1"/>
<xsd:enumeration value="Solution 2"/>
<xsd:enumeration value="Fluid (supercritical or subcritical phases)"/>
<xsd:enumeration value="Ideal gas"/>
<xsd:enumeration value="Gas"/>
<xsd:enumeration value="Air at 1 atmosphere"/>
</xsd:restriction>
</xsd:simpleType>
<xsd:simpleType name="ePresentation">
  <xsd:annotation>
    <xsd:documentation>Means of property presentation</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Direct value, X"/>
    <xsd:enumeration value="Difference between upper and lower temperature, X(T2)-X(T1)"/>
    <xsd:enumeration value="Difference between upper and lower pressure, X(P2)-X(P1)"/>
    <xsd:enumeration value="Mean between upper and lower temperature, [X(T2)+X(T1)]/2"/>
    <xsd:enumeration value="Difference with the reference state, X-X(REF)"/>
    <xsd:enumeration value="Ratio with the reference state, X/X(REF)"/>
    <xsd:enumeration value="Ratio of difference with the reference state to the reference state, [X-X(REF)]/X(REF)"/>
  </xsd:restriction>
</xsd:simpleType>
<!--
-->
<xsd:simpleType name="eRefStateType">
  <xsd:annotation>
    <xsd:documentation>Type of reference state</xsd:documentation>
  </xsd:annotation>
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="Reference phase with the same composition at fixed temperature and pressure"/>
    <xsd:enumeration value="Reference phase with the same composition, temperature and pressure"/>

```

```

    <xsd:enumeration value="Reference phase at fixed temperature and the same
pressure"/>
    <xsd:enumeration value="Reference phase at the same temperature and fixed
pressure"/>
    <xsd:enumeration value="Phase in equilibrium with primary phase at the same
temperature and pressure"/>
    <xsd:enumeration value="Pure components in the same proportion at the same
temperature and pressure"/>
    <xsd:enumeration value="Pure solvent at the temperature of the same phase
equilibrium"/>
        <xsd:enumeration value="Pure solvent at the same temperature and pressure"/>
        <xsd:enumeration value="Pure solute at the same temperature and pressure"/>
    </xsd:restriction>
</xsd:simpleType>
<!--

-->
<xsd:element name="RegNum">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nCASRNum" type="xsd:integer" minOccurs="0"/>
            <xsd:element name="nOrgNum" type="xsd:integer" minOccurs="0"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<!--

-->
<xsd:element name="Solvent">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element ref="RegNum" maxOccurs="unbounded"/>
        </xsd:sequence>
    </xsd:complexType>
</xsd:element>
<!--

-->
<xsd:complexType name="ConstraintVariableType">
    <xsd:choice>
        <xsd:element name="eTemperature">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">

```

```

<xsd:enumeration value="Temperature, K"/>
<xsd:enumeration value="Upper temperature, K"/>
<xsd:enumeration value="Lower temperature, K"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="ePressure">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Pressure, kPa"/>
<xsd:enumeration value="Partial pressure, kPa"/>
<xsd:enumeration value="Upper pressure, kPa"/>
<xsd:enumeration value="Lower pressure, kPa"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="eComponentComposition">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Mole fraction"/>
<xsd:enumeration value="Mass fraction"/>
<xsd:enumeration value="MolaLity, mol/kg"/>
<xsd:enumeration value="MolaRity, mol/dm3"/>
<xsd:enumeration value="Volume fraction"/>
<xsd:enumeration value="Moles per mass of solution, mol/kg"/>
<xsd:enumeration value="Mass per volume of solution, kg/m3"/>
<xsd:enumeration value="Mole ratio to solvent"/>
<xsd:enumeration value="Mass ratio to solvent"/>
<xsd:enumeration value="Volume ratio to solvent"/>
<xsd:enumeration value="Activity"/>
<xsd:enumeration value="Activity coefficient"/>
<xsd:enumeration value="Initial mole fraction"/>
<xsd:enumeration value="Initial mass fraction"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="eSolventComposition">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Solvent: Mole fraction"/>
<xsd:enumeration value="Solvent: Mass fraction"/>
<xsd:enumeration value="Solvent: Volume fraction"/>
<xsd:enumeration value="Solvent: MolaLity, mol/kg"/>

```

```

        <xsd:enumeration value="Solvent: Molarity, mol/dm3"/>
        <xsd:enumeration value="Solvent: Mole ratio to other component of binary
solvent"/>
        <xsd:enumeration value="Solvent: Mass ratio to other component of binary
solvent"/>
        <xsd:enumeration value="Solvent: Volume ratio to other component of binary
solvent"/>
        <xsd:enumeration value="Solvent: Moles per mass of solvent, mol/kg"/>
        <xsd:enumeration value="Solvent: Mass per volume of solvent, kg/m3"/>
    </xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="eMiscellaneous">
    <xsd:simpleType>
        <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Wavelength, nm"/>
            <xsd:enumeration value="Molar volume, m3/mol"/>
            <xsd:enumeration value="Specific volume, m3/kg"/>
            <xsd:enumeration value="Density, kg/m3"/>
            <xsd:enumeration value="Molar density, mol/m3"/>
            <xsd:enumeration value="Entropy, J/K/mol"/>
        </xsd:restriction>
    </xsd:simpleType>
</xsd:element>
</xsd:choice>
</xsd:complexType>
<!--
-->
<xsd:complexType name="ConstrDeviceSpecType">
    <xsd:sequence>
        <xsd:element name="sDeviceSpecEvaluator" type="xsd:string" minOccurs="0"/>
        <xsd:element name="eDeviceSpecMethod">
            <xsd:simpleType>
                <xsd:restriction base="xsd:string">
                    <xsd:enumeration value="Specified by the manufacturer"/>
                    <xsd:enumeration value="Certified or calibrated by a third party"/>
                    <xsd:enumeration value="Calibrated by the experimentalist"/>
                </xsd:restriction>
            </xsd:simpleType>
        </xsd:element>
        <xsd:element name="sDeviceSpecMethod" type="xsd:string" minOccurs="0"/>
        <xsd:element name="nDeviceSpecValue" type="xsd:float" minOccurs="0"/>
    </xsd:sequence>
</xsd:complexType>

```

```

<xsd:element name="nDeviceSpecLevOfConfid" type="xsd:float" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="PropVarDeviceSpecType">
<xsd:sequence>
<xsd:element name="sDeviceSpecEvaluator" type="xsd:string" minOccurs="0"/>
<xsd:element name="eDeviceSpecMethod">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Specified by the manufacturer"/>
<xsd:enumeration value="Certified or calibrated by a third party"/>
<xsd:enumeration value="Calibrated by the experimentalist"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sDeviceSpecMethod" type="xsd:string" minOccurs="0"/>
<xsd:element name="nDeviceSpecLevOfConfid" type="xsd:float" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="ConstrRepeatabilityType">
<xsd:sequence>
<xsd:element name="sRepeatEvaluator" type="xsd:string" minOccurs="0"/>
<xsd:element name="eRepeatMethod">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Standard deviation of a single value (biased)"/>
<xsd:enumeration value="Standard deviation of a single value (unbiased)"/>
<xsd:enumeration value="Standard deviation of the mean"/>
<xsd:enumeration value="Other"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sRepeatMethod" type="xsd:string" minOccurs="0"/>
<xsd:element name="nRepeatValue" type="xsd:float" minOccurs="0"/>
<xsd:element name="nRepetitions" type="xsd:integer" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>

```

```

<!--
-->
<xsd:complexType name="PropVarRepeatabilityType">
  <xsd:sequence>
    <xsd:element name="sRepeatEvaluator" type="xsd:string" minOccurs="0"/>
    <xsd:element name="eRepeatMethod">
      <xsd:simpleType>
        <xsd:restriction base="xsd:string">
          <xsd:enumeration value="Standard deviation of a single value (biased)"/>
          <xsd:enumeration value="Standard deviation of a single value (unbiased)"/>
          <xsd:enumeration value="Standard deviation of the mean"/>
          <xsd:enumeration value="Other"/>
        </xsd:restriction>
      </xsd:simpleType>
    </xsd:element>
    <xsd:element name="sRepeatMethod" type="xsd:string" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>
<!--
-->
<xsd:element name="CurveDev">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nCurveDevAssessNum" type="xsd:integer"/>
      <xsd:element name="sCurveDevEvaluator" type="xsd:string" minOccurs="0"/>
      <xsd:element name="sCurveSpec" type="xsd:string"/>
      <xsd:element name="nCurveRmsDevValue" type="xsd:float" minOccurs="0"/>
      <xsd:element name="nCurveRmsRelativeDevValue" type="xsd:float"
minOccurs="0"/>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<!--
-->
<xsd:complexType name="ConstrUncertaintyType">
  <xsd:sequence>
    <xsd:element name="sUncertEvaluator" type="xsd:string" minOccurs="0"/>
    <xsd:element name="sUncertEvalMethod" type="xsd:string" minOccurs="0"/>
    <xsd:element name="nStdUncertValue" type="xsd:float" minOccurs="0"/>
    <xsd:element name="nCoverageFactor" type="xsd:float" minOccurs="0"/>

```

```

<xsd:element name="nExpandUncertValue" type="xsd:float" minOccurs="0"/>
<xsd:element name="nUncertLevOfConfid" type="xsd:float" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="PropVarUncertaintyType">
<xsd:sequence>
<xsd:element name="nUncertAssessNum" type="xsd:integer"/>
<xsd:element name="sUncertEvaluator" type="xsd:string" minOccurs="0"/>
<xsd:element name="sUncertEvalMethod" type="xsd:string" minOccurs="0"/>
<xsd:element name="nCoverageFactor" type="xsd:float" minOccurs="0"/>
<xsd:element name="nUncertLevOfConfid" type="xsd:float" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:complexType name="AsymUncertType">
<xsd:sequence>
<xsd:element name="nPositiveValue" type="xsd:float" minOccurs="0"/>
<xsd:element name="nNegativeValue" type="xsd:float" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
<!--

-->
<xsd:element name="CombinedUncertainty">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nCombUncertAssessNum" type="xsd:integer"/>
<xsd:element name="sCombUncertEvaluator" type="xsd:string" minOccurs="0"/>
<xsd:element name="eCombUncertEvalMethod">
<xsd:simpleType>
<xsd:restriction base="xsd:string">
<xsd:enumeration value="Propagation of evaluated standard uncertainties"/>
<xsd:enumeration value="Comparison with reference property values"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sCombUncertEvalMethod" type="xsd:string"
minOccurs="0"/>

```

```

<xsd:element name="nCombCoverageFactor" type="xsd:float" minOccurs="0"/>
<xsd:element name="nCombUncertLevOfConfid" type="xsd:float"
minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<!--
-->
<xsd:element name="NumValues">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="VariableValue" minOccurs="0" maxOccurs="unbounded">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nVarNumber" type="xsd:integer"/>
<xsd:element name="nVarValue" type="xsd:float"/>
<xsd:element name="nVarDigits" type="xsd:integer"/>
<xsd:element name="VarUncertainty" minOccurs="0"
maxOccurs="unbounded">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nUncertAssessNum" type="xsd:integer"/>
<xsd:element name="nStdUncertValue" type="xsd:float"
minOccurs="0"/>
<xsd:element name="nExpandUncertValue" type="xsd:float"
minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="VarRepeatability" minOccurs="0">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nVarRepeatValue" type="xsd:float"/>
<xsd:element name="nRepetitions" type="xsd:integer"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="nVarDeviceSpecValue" type="xsd:float"
minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>

```

```

<xsd:element name="PropertyValue" maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nPropNumber" type="xsd:integer"/>
      <xsd:choice>
        <xsd:sequence>
          <xsd:element name="nPropValue" type="xsd:float"/>
          <xsd:element name="nPropDigits" type="xsd:integer"/>
        </xsd:sequence>
      <xsd:element name="PropLimit">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:choice>
              <xsd:element name="nPropUpperLimitValue" type="xsd:float"/>
              <xsd:element name="nPropLowerLimitValue" type="xsd:float"/>
            </xsd:choice>
            <xsd:element name="nPropLimitDigits" type="xsd:integer"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
    </xsd:choice>
  <xsd:element name="CombinedUncertainty" minOccurs="0"
maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nCombUncertAssessNum" type="xsd:integer"/>
      <xsd:choice>
        <xsd:sequence>
          <xsd:element name="nCombStdUncertValue" type="xsd:float"
minOccurs="0"/>
          <xsd:element name="nCombExpandUncertValue" type="xsd:float"
minOccurs="0"/>
        </xsd:sequence>
        <xsd:sequence>
          <xsd:element name="AsymCombStdUncert" type="AsymUncertType"
minOccurs="0"/>
          <xsd:element name="AsymCombExpandUncert"
type="AsymUncertType" minOccurs="0"/>
        </xsd:sequence>
      </xsd:choice>
    </xsd:sequence>
  </xsd:complexType>
</xsd:element>

```

```

<xsd:element name="PropUncertainty" minOccurs="0"
maxOccurs="unbounded">
    <xsd:complexType>
        <xsd:sequence>
            <xsd:element name="nUncertAssessNum" type="xsd:integer"/>
            <xsd:choice>
                <xsd:sequence>
                    <xsd:element name="nStdUncertValue" type="xsd:float"
minOccurs="0"/>
                    <xsd:element name="nExpandUncertValue" type="xsd:float"
minOccurs="0"/>
                </xsd:sequence>
                <xsd:sequence>
                    <xsd:element name="AsymStdUncert" type="AsymUncertType"
minOccurs="0"/>
                    <xsd:element name="AsymExpandUncert" type="AsymUncertType"
minOccurs="0"/>
                </xsd:sequence>
                <xsd:choice>
                    </xsd:sequence>
                    </xsd:choice>
                </xsd:sequence>
            </xsd:complexType>
        </xsd:element>
        <xsd:element name="PropRepeatability" minOccurs="0">
            <xsd:complexType>
                <xsd:sequence>
                    <xsd:element name="nPropRepeatValue" type="xsd:float"/>
                    <xsd:element name="nRepetitions" type="xsd:integer"/>
                </xsd:sequence>
            </xsd:complexType>
        </xsd:element>
        <xsd:element name="nPropDeviceSpecValue" type="xsd:float"
minOccurs="0"/>
        <xsd:element name="CurveDev" minOccurs="0" maxOccurs="unbounded">
            <xsd:complexType>
                <xsd:sequence>
                    <xsd:element name="nCurveDevAssessNum" type="xsd:integer"/>
                    <xsd:element name="nCurveDevValue" type="xsd:float"/>
                </xsd:sequence>
            </xsd:complexType>
        </xsd:element>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>

```

```

    </xsd:sequence>
  </xsd:complexType>
</xsd:element>
<!--

-->
<xsd:element name="CriticalEvaluation">
  <xsd:complexType>
    <xsd:choice>
      <xsd:element name="SingleProp">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="sEvalSinglePropDescription" type="xsd:string"
minOccurs="0"/>
            <xsd:element name="EvalSinglePropRef" type="CitationType"
minOccurs="0" maxOccurs="unbounded"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="MultiProp">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="sEvalMultiPropList" type="xsd:string" minOccurs="0"/>
            <xsd:element name="sEvalMultiPropDescription" type="xsd:string"
minOccurs="0"/>
            <xsd:element name="EvalMultiPropRef" type="CitationType" minOccurs="0"
maxOccurs="unbounded"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
      <xsd:element name="EquationOfState">
        <xsd:complexType>
          <xsd:sequence>
            <xsd:element name="sEvalEOSName" type="xsd:string" minOccurs="0"/>
            <xsd:element name="sEvalEOSDescription" type="xsd:string"
minOccurs="0"/>
            <xsd:element name="EvalEOSRef" type="CitationType" minOccurs="0"
maxOccurs="unbounded"/>
          </xsd:sequence>
        </xsd:complexType>
      </xsd:element>
    </xsd:choice>
  </xsd:complexType>

```

```

</xsd:element>
<!--

-->
<xsd:element name="Prediction">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="ePredictionType">
        <xsd:simpleType>
          <xsd:restriction base="xsd:string">
            <xsd:enumeration value="Ab initio"/>
            <xsd:enumeration value="Molecular dynamics"/>
            <xsd:enumeration value="Semiempirical quantum methods"/>
            <xsd:enumeration value="Molecular mechanics"/>
            <xsd:enumeration value="Statistical mechanics"/>
            <xsd:enumeration value="Corresponding states"/>
            <xsd:enumeration value="Correlation"/>
            <xsd:enumeration value="Group contribution"/>
          </xsd:restriction>
        </xsd:simpleType>
      </xsd:element>
      <xsd:element name="sPredictionMethodName" type="xsd:string"
minOccurs="0"/>
        <xsd:element name="sPredictionMethodDescription" type="xsd:string"
minOccurs="0"/>
          <xsd:element name="PredictionMethodRef" type="CitationType" minOccurs="0"
maxOccurs="unbounded"/>
        </xsd:sequence>
      </xsd:complexType>
    </xsd:element>
  <!--

-->
<xsd:element name="Equation">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:choice>
        <xsd:element name="eEqName">
          <xsd:simpleType>
            <xsd:restriction base="xsd:string">
              <xsd:enumeration value="ThermoML.Antoine"/>
              <xsd:enumeration value="ThermoML.CustomExpansion"/>
              <xsd:enumeration value="ThermoML.Helmholtz3General.EOS"/>

```

```

<xsd:enumeration value="ThermoML.Helmholtz4General.EOS"/>
<xsd:enumeration value="ThermoML.WagnerLinear.VaporPressure"/>
<xsd:enumeration value="ThermoML.Wagner25Linear.VaporPressure"/>
<xsd:enumeration value="ThermoML.Wagner36Linear.VaporPressure"/>
<xsd:enumeration value="ThermoML.PolynomialExpansion"/>
<xsd:enumeration value="ThermoML.SpanWagner12Nonpolar.EOS"/>
<xsd:enumeration value="ThermoML.SpanWagner12Polar.EOS"/>
</xsd:restriction>
</xsd:simpleType>
</xsd:element>
<xsd:element name="sEqName" type="xsd:string"/>
</xsd:choice>
<xsd:element name="urlMathSource" type="xsd:string"/>
<xsd:element name="EqProperty" minOccurs="0" maxOccurs="unbounded">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nPropNumber" type="xsd:integer"/>
<xsd:element name="sEqSymbol" type="xsd:string"/>
<xsd:element name="nEqPropIndex" type="xsd:integer" minOccurs="0"
maxOccurs="unbounded"/>
<xsd:element name="sOtherPropUnit" type="xsd:string" minOccurs="0"/>
<xsd:element name="nEqPropRangeMin" type="xsd:float" minOccurs="0"/>
<xsd:element name="nEqPropRangeMax" type="xsd:float" minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="EqConstraint" minOccurs="0" maxOccurs="unbounded">
<xsd:complexType>
<xsd:sequence>
<xsd:element name="nConstraintNumber" type="xsd:integer"/>
<xsd:element name="sEqSymbol" type="xsd:string"/>
<xsd:element name="nEqConstraintIndex" type="xsd:integer" minOccurs="0"
maxOccurs="unbounded"/>
<xsd:element name="sOtherConstraintUnit" type="xsd:string"
minOccurs="0"/>
<xsd:element name="nEqConstraintRangeMin" type="xsd:float"
minOccurs="0"/>
<xsd:element name="nEqConstraintRangeMax" type="xsd:float"
minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="EqVariable" minOccurs="0" maxOccurs="unbounded">

```

```

<xsd:complexType>
  <xsd:sequence>
    <xsd:element name="nVarNumber" type="xsd:integer"/>
    <xsd:element name="sEqSymbol" type="xsd:string"/>
    <xsd:element name="nEqVarIndex" type="xsd:integer" minOccurs="0"
maxOccurs="unbounded"/>
    <xsd:element name="sOtherVarUnit" type="xsd:string" minOccurs="0"/>
    <xsd:element name="nEqVarRangeMin" type="xsd:float" minOccurs="0"/>
    <xsd:element name="nEqVarRangeMax" type="xsd:float" minOccurs="0"/>
  </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="EqParameter" minOccurs="0" maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nEqParNumber" type="xsd:integer" minOccurs="0"/>
      <xsd:element name="sEqParSymbol" type="xsd:string"/>
      <xsd:element name="nEqParIndex" type="xsd:integer" minOccurs="0"
maxOccurs="unbounded"/>
      <xsd:element name="nEqParValue" type="xsd:float"/>
      <xsd:element name="nEqParDigits" type="xsd:integer"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="EqConstant" minOccurs="0" maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="sEqConstantSymbol" type="xsd:string"/>
      <xsd:element name="nEqConstantIndex" type="xsd:integer" minOccurs="0"
maxOccurs="unbounded"/>
      <xsd:element name="nEqConstantValue" type="xsd:float"/>
      <xsd:element name="nEqConstantDigits" type="xsd:integer"/>
    </xsd:sequence>
</xsd:complexType>
</xsd:element>
<xsd:element name="Covariance" minOccurs="0" maxOccurs="unbounded">
  <xsd:complexType>
    <xsd:sequence>
      <xsd:element name="nEqParNumber1" type="xsd:integer"/>
      <xsd:element name="nEqParNumber2" type="xsd:integer"/>
      <xsd:element name="nCovarianceValue" type="xsd:float"/>
    </xsd:sequence>
</xsd:complexType>

```

```
</xsd:element>
<xsd:element name="nCovarianceLevOfConfid" type="xsd:float"
minOccurs="0"/>
</xsd:sequence>
</xsd:complexType>
</xsd:element>
</xsd:schema>
```

Literature Cited

- (1) Steele, W. V., Chirico, R. D., Cowell, A. B., Nguyen, A., Knipmeyer, S. E. Possible precursors and products of deep hydrodesulfurization of gasoline and distillate fuels. Part 2. The thermodynamic properties of 2,3-dihydrobenzo[b]thiophene. *J. Chem. Thermodyn.* **2003**, 35, 1253-1276.
- (2) Chirico, R. D., Knipmeyer, S. E., Nguyen, A., Steele, W. V. Thermodynamic properties of the methylpyridines. Part 2. Vapor pressures, heat capacities, critical properties, derived thermodynamic functions between the temperatures 250 K and 560 K, and equilibrium isomer distributions for all temperatures ≥ 250 K. *J. Chem. Thermodyn.* **1999**, 31, 339-378.